REMARKS

Reconsideration is respectfully requested. Claims 1, 4, 6, 9, 10, and 18-24 are pending. Claims 2-3, 5, 7-8, and 11-17 are canceled. New claim 24 is added. Claims 1, 4, 9 and 19 are amended. Cancellation and amendment of the claims does not affect inventorship.

Applicants have not dedicated or abandoned any unclaimed subject matter and moreover have not acquiesced to any rejections made by the Patent Office. Applicants reserve the right to pursue prosecution of any presently excluded claim embodiments in future continuation and/or divisional applications.

Claim Amendments

Claims 1, 4, 9 and 19 are amended. New claim 24 has been added. Support is found in the specification, for example, in paragraphs [00178] and [00183].

Objections to the Specification

The Examiner has objected to the Specification because of certain informalities, each of which are addressed separately below:

Firstly, the specification is objected to because of the inappropriate use of SEQ ID NOs and number of residues that do not correspond to the SEQ ID NOs. The Examiner specifically cites to paragraph [00180] in connection with the objection. Applicants respectfully direct the Examiner's attention to the Amendment in Response to Official Action filed on June 30, 2006, wherein Applicants amended several portions of the Specification, and specifically requested that paragraph [00180] be deleted. Thus, the objection raised by the Examiner with respect to paragraph [00180] is moot in light of its deletion.

Secondly, the Examiner refers to informalities in Example 2, i.e., paragraph [00183] of the Specification. The Examiner is referred to the Amendment in Response to Official Action filed on June 30, 2006, wherein Applicants amended paragraphs [00178] and [00183]. The amendment specifically states that SEQ ID NO:2 comprises a coding sequence for a N-terminal His-tag coupled to full length IspA, and that SEQ ID NO:2 is expressed in the pSX28 vector to generate a fusion protein of the full length IspA with a non-cleavable amino-terminal six histidine tag, i.e., SEQ ID NO:1. The foregoing amendment in conjunction with the deletion of paragraph [00180] renders the objection moot.

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Thirdly, the Examiner has raised an objection with respect to a typographical error in the Oath and Declaration concerning the spelling of the first inventor's name. The first inventor's name is correctly spelled as Alexei Brooun in the Oath and Declaration; whilst being incorrectly spelled in the Hosfield et al. (2004) publication. Thus, there is no error in the Oath and Declaration.

In light of the above arguments, the Examiner is requested to withdraw the objections to the Specification.

Objections to the Drawings

In response to the objection to the drawings raised by the Examiner, Applicants have submitted corrected annotated and replacement drawing sheets for Figure 3, in conjunction with this paper.

Claim Rejection Under 35 U.S.C. § 112

Indefiniteness

Claims 1, 4 and 16 are rejected for failing to particularly and distinctly claim the subject matter which applicant regards as the invention. Claim 16 has been canceled and its claim limitation is now incorporated in claims 1 and 4. Claims 1 and 4, as amended, are directed to a composition comprising a protein in crystalline form, wherein the protein consists of residues 1-314 of SEQ ID NO:1, and wherein the **protein crystal** has a crystal lattice in a $P4_122$ space group and unit cell dimensions, +/- 5%, of a=88.80Å b=88.80Å and c=174.99Å, $\alpha=\beta=\gamma=90$ (emphasis added). Applicants believe that the scope of claims 1 and 4 as currently recited are clear on their face, and therefore respectfully request the withdrawal of the instant rejection.

Written Description and Enablement

Claims 1,4,6, 9, 10, 16 and 18-23 stand rejected under 35 U.S.C. § 112, first paragraph as failing to comply with the written description and enablement requirement. Applicants respectfully traverse.

Claim 16 has been cancelled, thereby rendering the rejections with respect to this claim moot.

Applicants respectfully direct the Examiner to M.P.E.P. 2163, which states:

The written description requirement for a claimed genus may be satisfied through sufficient description of a representative number of species by actual reduction to practice.

The Examiner states that:

> While the structure and function of one species of said genera of IspA are disclosed in the specification, the common structural characteristics of species that define said genera are not described.

Applicants respectfully disagree. Claim 1 as amended recites a protein crystal having a crystal lattice in a $P4_122$ space group and unit cell dimensions, +/- 5%, of a=88.80Å b=88.80Å and c=174.99Å, $\alpha=\beta=\gamma=90$. Thus, it claims a genus method to grow this specific crystal of a protein. As stated in M.P.E.P. 2163:

> A "representative number of species" means that the species which are adequately described are representative of the entire genus.

> ....

> What constitutes a "representative number" is an inverse function of the skill and knowledge in the art. Satisfactory disclosure of a "representative number" depends on whether one of skill in the art would recognize that the applicant was in possession of the necessary common attributes or features of the elements possessed by the members of the genus in view of the species disclosed.... Description of a representative number of species does not require the description to be of such specificity that it would provide individual support for each species that the genus embraces.

Moreover, as the Examiner can appreciate, at the beginning of this new millennium, the time the instant application was filed, "the skill and knowledge in the art" required for growing crystal had come a long way from the early age of crystallography, or even a decade before then. Kits for large scale screening were widely commercially available, and methods and equipments for robotic large scale screening have been developed by several entities. Due to these developments, large scale screening with minimal amount of protein for conditions to grow crystals became routine, particularly in the industry.

A simple search on Google Scholar for references relating to protein crystallization methods yielded in excess of 30,000 hits most of which had a publication date prior to the filing date of the instant application in 2003. A sampling of the references is provided below. Therefore, it is quite clear that the level of skill in the art was high, with respect to crystallization methods, at the time the application was filed. Hence, a skilled artisan would have been more than capable of arriving at the conditions for crystallization of a protein consisting of "residues 1-314 of SEQ ID NO:1."

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U.S. Serial No.: 10/651,668
Filing Date: August 28, 2003

List of References

High-throughput protein crystallization - RC Stevens - Curr. Opin. Struct. Biol, **2000**

Overview of Protein Crystallization Methods- PC Weber - Methods in enzymology, **1997**

Comparative studies of protein crystallization by vapour-diffusion and microbatch techniques - NE Chayen - Acta Crystallogr D Biol Crystallogr, **1998**

An approach to rapid protein crystallization using nanodroplets - DC Uber, EW Cornell, RA Nordmeyer, WF Kolbe, J Jin - J Appl Crystallogr, **2002**

An automated system for micro-batch protein crystallization and screening - NE Chayen, PD Shaw Stewart, DL Maeder, DM Blow - Journal of Applied Crystallography, **1990**

Protein crystallization for genomics: towards high-throughput optimization techniques - NE Chayen, E Saridakis - Acta Crystallographica Section D Biological Crystallography, **2002**

Protein Crystallization - SD Durbin, G Feher - Annual Review of Physical Chemistry, **1996**

System for Evaluating Protein Crystallization Conditions by Microbatch and Vapor-Diffusion Methods - B Zheng, JD Tice, LS Roach, RF Ismagilov - Angewandte Chemie International Edition, 2004

Principles of Protein X-Ray Crystallography- J Drenth - **1999**

Screening of protein crystallization conditions on a microfluidic chip using nanoliter-size droplets - B Zheng, LS Roach, RF Ismagilov - J Am Chem Soc, **2003**

Protein interactions and crystallization- DF ROSENBAUM, CF ZUKOSKI - Journal of crystal growth, **1996**.

Protein Crystallization: Micro Techniques Involving Vapor Diffusion- DR Davies, DM Segal - Methods Enzymol, **1971**

As such, at the time the instant application was filed, "the skill and knowledge in the art" had grown into a stage that it was not necessary to disclose each and every condition, foreseeable or unforeseeable, to meet the ""representative number" requirement. Description of a representative number of conditions to grow the claimed specific crystal does not require the description of such specificity each growing condition. The wide range of crystallization conditions disclosed by the present invention is sufficient to provide guidance to further explore for new conditions to grow the claimed crystal.

As such, at the time the instant application was filed, "the skill and knowledge in the art" had grown into a stage that it was not necessary to disclose each and every condition, foreseeable or

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unforeseeable, to meet the ""representative number" requirement. Description of a representative number of conditions to grow the claimed specific crystal does not require the description of such specificity each growing condition. The wide range of crystallization conditions disclosed by the present invention is sufficient to provide guidance to further explore for new conditions to grow the claimed crystal.

Applicants further submit that a sufficient "representative number" of conditions - the conditions to grow the specific crystal as recited in claim 6- have been provided by the instant application. The specification discloses that the Applicants have undertaken "systematic broad screening crystallization trials on an IspA complex using the sitting drop techniques" to obtain conditions that appear to produce precipitate and/or crystals. These conditions are used for fine screening for optimal conditions. *See* paragraphs [0086] and [0087]. These experiments led to a thorough understanding of how crystallization conditions affect IspA crystallization, and a series of crystallization conditions were identified that maybe used to for crystals comprising IspA. These conditions are summarized in Table 8. The specification further discloses in details one of the crystals obtained under one of the disclosed conditions. *See* Example 2. Therefore, the Applicants have disclosed a range of conditions that can be used to grow the claimed specific crystal.

Thus, at the time of the filing, Applicants not only were in possession of the claimed genus method, but also provided sufficient guidance to enable a skilled artisan to practice the claimed method without undue experimentation. As such, the rejection is improper and should be withdrawn.

CONCLUSION

Applicants respectfully submit that the claims are now in condition for allowance and early notification to that effect is respectfully requested. If the Examiner feels there are further unresolved issues, the Examiner is respectfully requested to phone the undersigned at (415) 442-1000.

Respectfully submitted,

Dated: _August 6, 2007_   By: _____

Customer Number: 67374   Lekha Gopalakrishnan, Reg. No. 46,733
Morgan, Lewis & Bockius LLP
One Market, Spear Street Tower   _Filed Under 37 C.F.R. § 1.34_
San Francisco, CA 94105
Telephone: (415) 442-1000   On behalf of:
Facsimile: (415) 442-1001   Robin M. Silva, Reg. No. 38,304

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FIGURE 3AA

LEGEND

Column headings from left to right are (A)'Atom Number', (B)'Atom Type', (C)'Amino Acid', (D)'Chain Identifier', (E)'Amino Acid Number', (F)'X Coordinate', (G)'Y Coordinate', (H)'Z Coordinate', (I)'Occupancy' (OCC) and (J)'B factor'.

A	B	C	D	E	F	G	H	I	J
1	N	MET	A	16	65.564	50.628	-5.933	1.00	45.23
3	CA	MET	A	16	65.166	51.178	-7.255	1.00	44.87
5	CB	MET	A	16	64.933	50.049	-8.267	1.00	45.30
8	CG	MET	A	16	65.153	50.446	-9.726	1.00	47.01
11	SD	MET	A	16	66.181	49.252	-10.631	1.00	50.95
12	CE	MET	A	16	64.933	48.059	-11.220	1.00	50.52
16	C	MET	A	16	63.907	52.030	-7.120	1.00	43.94
17	O	MET	A	16	63.880	53.159	-7.610	1.00	44.23
20	N	ASP	A	17	62.875	51.491	-6.466	1.00	42.41
22	CA	ASP	A	17	61.591	52.188	-6.366	1.00	41.35
24	CB	ASP	A	17	60.409	51.226	-6.459	1.00	41.74
27	CG	ASP	A	17	59.134	51.926	-6.899	1.00	43.33
28	OD1	ASP	A	17	58.448	52.535	-6.037	1.00	46.33
29	OD2	ASP	A	17	58.753	51.939	-8.093	1.00	45.52
30	C	ASP	A	17	61.486	52.990	-5.079	1.00	39.80
31	O	ASP	A	17	61.195	52.441	-4.005	1.00	38.54
32	N	PHE	A	18	61.672	54.298	-5.210	1.00	38.05
34	CA	PHE	A	18	61.858	55.146	-4.050	1.00	36.90
36	CB	PHE	A	18	62.429	56.514	-4.427	1.00	36.92
39	CG	PHE	A	18	63.016	57.233	-3.260	1.00	36.41
40	CD1	PHE	A	18	64.116	56.707	-2.609	1.00	37.05
42	CE1	PHE	A	18	64.658	57.340	-1.502	1.00	36.55
44	CZ	PHE	A	18	64.098	58.493	-1.036	1.00	36.07
46	CE2	PHE	A	18	62.988	59.025	-1.664	1.00	36.56
48	CD2	PHE	A	18	62.442	58.392	-2.768	1.00	36.65
50	C	PHE	A	18	60.632	55.314	-3.158	1.00	35.80
51	O	PHE	A	18	60.769	55.198	-1.949	1.00	35.17
52	N	PRO	A	19	59.456	55.618	-3.712	1.00	34.90
53	CA	PRO	A	19	58.239	55.676	-2.889	1.00	34.06
55	CB	PRO	A	19	57.123	55.861	-3.924	1.00	34.29
58	CG	PRO	A	19	57.782	56.558	-5.047	1.00	34.27
61	CD	PRO	A	19	59.176	55.993	-5.114	1.00	34.77
64	C	PRO	A	19	58.008	54.418	-2.039	1.00	33.38
65	O	PRO	A	19	57.585	54.564	-0.895	1.00	32.65
66	N	GLN	A	20	58.279	53.228	-2.579	1.00	32.48
68	CA	GLN	A	20	58.126	51.981	-1.815	1.00	32.23
70	CB	GLN	A	20	58.188	50.746	-2.732	1.00	32.68
73	CG	GLN	A	20	56.883	50.493	-3.534	1.00	35.01
76	CD	GLN	A	20	56.611	49.011	-3.811	1.00	39.06
77	OE1	GLN	A	20	55.463	48.546	-3.685	1.00	41.57
78	NE2	GLN	A	20	57.654	48.270	-4.193	1.00	39.95
81	C	GLN	A	20	59.177	51.869	-0.700	1.00	30.90
82	O	GLN	A	20	58.892	51.363	0.379	1.00	30.03

FIGURE 3 (Cont.)AB

A	B	C	D	E	F	G	H	I	J
83	N	GLN	A	21	60.385	52.351	-0.959	1.00	29.82
85	CA	GLN	A	21	61.426	52.370	0.058	1.00	29.68
87	CB	GLN	A	21	62.783	52.738	-0.560	1.00	29.82
90	CG	GLN	A	21	63.366	51.647	-1.494	1.00	31.98
93	CD	GLN	A	21	63.920	50.425	-0.746	1.00	34.89
94	OE1	GLN	A	21	64.483	49.512	-1.360	1.00	36.76
95	NE2	GLN	A	21	63.762	50.412	0.572	1.00	37.29
98	C	GLN	A	21	61.065	53.323	1.204	1.00	28.61
99	O	GLN	A	21	61.214	52.973	2.372	1.00	28.03
100	N	LEU	A	22	60.588	54.513	0.863	1.00	27.80
102	CA	LEU	A	22	60.120	55.472	1.848	1.00	27.76
104	CB	LEU	A	22	59.582	56.740	1.169	1.00	28.15
107	CG	LEU	A	22	60.595	57.714	0.543	1.00	29.56
109	CD1	LEU	A	22	59.880	58.764	-0.297	1.00	30.48
113	CD2	LEU	A	22	61.447	58.392	1.611	1.00	30.42
117	C	LEU	A	22	59.036	54.861	2.736	1.00	27.31
118	O	LEU	A	22	59.099	54.975	3.950	1.00	26.43
119	N	GLU	A	23	58.057	54.185	2.145	1.00	27.14
121	CA	GLU	A	23	56.973	53.627	2.952	1.00	27.44
123	CB	GLU	A	23	55.760	53.232	2.101	1.00	28.34
126	CG	GLU	A	23	54.798	52.234	2.759	1.00	31.44
129	CD	GLU	A	23	53.961	52.789	3.912	1.00	35.82
130	OE1	GLU	A	23	52.791	52.370	4.024	1.00	38.87
131	OE2	GLU	A	23	54.448	53.597	4.738	1.00	38.87
132	C	GLU	A	23	57.465	52.462	3.805	1.00	26.15
133	O	GLU	A	23	57.040	52.322	4.949	1.00	25.29
134	N	ALA	A	24	58.357	51.642	3.254	1.00	25.31
136	CA	ALA	A	24	59.018	50.578	4.013	1.00	24.72
138	CB	ALA	A	24	60.019	49.847	3.153	1.00	25.46
142	C	ALA	A	24	59.728	51.160	5.230	1.00	24.33
143	O	ALA	A	24	59.610	50.636	6.331	1.00	23.33
144	N	CYS	A	25	60.438	52.263	5.025	1.00	23.38
146	CA	CYS	A	25	61.130	52.944	6.115	1.00	23.00
148	CB	CYS	A	25	62.029	54.056	5.578	1.00	23.11
151	SG	CYS	A	25	62.861	54.980	6.885	1.00	21.11
152	C	CYS	A	25	60.147	53.499	7.162	1.00	22.39
153	O	CYS	A	25	60.368	53.344	8.351	1.00	22.44
154	N	VAL	A	26	59.051	54.105	6.725	1.00	22.24
156	CA	VAL	A	26	58.056	54.638	7.651	1.00	22.18
158	CB	VAL	A	26	56.889	55.349	6.902	1.00	22.57
160	CG1	VAL	A	26	55.697	55.610	7.815	1.00	22.85
164	CG2	VAL	A	26	57.368	56.650	6.293	1.00	22.19
168	C	VAL	A	26	57.534	53.530	8.580	1.00	21.91
169	O	VAL	A	26	57.440	53.722	9.789	1.00	21.65
170	N	LYS	A	27	57.235	52.369	8.011	1.00	21.41
172	CA	LYS	A	27	56.741	51.236	8.779	1.00	21.24
174	CB	LYS	A	27	56.273	50.127	7.836	1.00	22.15
177	CG	LYS	A	27	54.982	50.454	7.081	1.00	24.03
180	CD	LYS	A	27	54.467	49.210	6.340	1.00	28.62
183	CE	LYS	A	27	53.133	49.458	5.596	1.00	31.91
186	NZ	LYS	A	27	53.166	48.924	4.184	1.00	33.67
190	C	LYS	A	27	57.798	50.693	9.737	1.00	20.33

FIGURE 3 (Cont.)AC

A	B	C	D	E	F	G	H	I	J
191	O	LYS	A	27	57.499	50.428	10.910	1.00	19.84
192	N	GLN	A	28	59.022	50.536	9.244	1.00	19.37
194	CA	GLN	A	28	60.116	50.039	10.073	1.00	19.22
196	CB	GLN	A	28	61.413	49.892	9.264	1.00	19.05
199	CG	GLN	A	28	62.596	49.326	10.078	1.00	19.21
202	CD	GLN	A	28	62.485	47.814	10.392	1.00	20.65
203	OE1	GLN	A	28	63.076	47.320	11.375	1.00	22.34
204	NE2	GLN	A	28	61.792	47.087	9.537	1.00	16.09
207	C	GLN	A	28	60.340	50.985	11.258	1.00	18.67
208	O	GLN	A	28	60.392	50.549	12.386	1.00	18.19
209	N	ALA	A	29	60.465	52.278	10.985	1.00	18.55
211	CA	ALA	A	29	60.748	53.271	12.026	1.00	18.70
213	CB	ALA	A	29	61.022	54.625	11.403	1.00	18.98
217	C	ALA	A	29	59.626	53.382	13.036	1.00	19.64
218	O	ALA	A	29	59.875	53.535	14.238	1.00	19.64
219	N	ASN	A	30	58.386	53.300	12.564	1.00	19.52
221	CA	ASN	A	30	57.232	53.369	13.464	1.00	19.96
223	CB	ASN	A	30	55.920	53.446	12.688	1.00	19.83
226	CG	ASN	A	30	55.652	54.816	12.118	1.00	22.13
227	OD1	ASN	A	30	56.322	55.792	12.458	1.00	23.82
228	ND2	ASN	A	30	54.638	54.904	11.249	1.00	23.36
231	C	ASN	A	30	57.177	52.190	14.405	1.00	19.86
232	O	ASN	A	30	56.847	52.343	15.573	1.00	19.83
233	N	GLN	A	31	57.474	51.010	13.878	1.00	20.51
235	CA	GLN	A	31	57.584	49.779	14.679	1.00	21.34
237	CB	GLN	A	31	57.921	48.608	13.760	1.00	21.77
240	CG	GLN	A	31	57.882	47.246	14.412	1.00	24.92
243	CD	GLN	A	31	58.025	46.137	13.385	1.00	29.08
244	OE1	GLN	A	31	59.120	45.918	12.832	1.00	33.06
245	NE2	GLN	A	31	56.929	45.446	13.112	1.00	31.52
248	C	GLN	A	31	58.683	49.902	15.737	1.00	21.05
249	O	GLN	A	31	58.488	49.550	16.899	1.00	20.55
250	N	ALA	A	32	59.839	50.384	15.310	1.00	20.90
252	CA	ALA	A	32	60.957	50.629	16.213	1.00	21.59
254	CB	ALA	A	32	62.129	51.176	15.451	1.00	21.36
258	C	ALA	A	32	60.539	51.598	17.315	1.00	21.65
259	O	ALA	A	32	60.696	51.304	18.475	1.00	22.05
260	N	LEU	A	33	59.999	52.750	16.940	1.00	22.61
262	CA	LEU	A	33	59.575	53.760	17.906	1.00	23.19
264	CB	LEU	A	33	58.931	54.937	17.175	1.00	23.47
267	CG	LEU	A	33	59.879	55.966	16.574	1.00	24.21
269	CD1	LEU	A	33	59.165	56.759	15.502	1.00	24.68
273	CD2	LEU	A	33	60.391	56.887	17.685	1.00	26.09
277	C	LEU	A	33	58.555	53.183	18.890	1.00	24.35
278	O	LEU	A	33	58.659	53.391	20.094	1.00	23.66
279	N	SER	A	34	57.567	52.471	18.356	1.00	25.27
281	CA	SER	A	34	56.513	51.879	19.172	1.00	26.76
283	CB	SER	A	34	55.480	51.162	18.295	1.00	27.01
286	OG	SER	A	34	54.789	52.077	17.470	1.00	28.06
288	C	SER	A	34	57.070	50.896	20.194	1.00	27.73
289	O	SER	A	34	56.597	50.849	21.316	1.00	28.77
290	N	ARG	A	35	58.071	50.117	19.802	1.00	28.38

FIGURE 3 (Cont.)AD

A	B	C	D	E	F	G	H	I	J
292	CA	ARG	A	35	58.649	49.117	20.688	1.00	29.15
294	CB	ARG	A	35	59.580	48.182	19.915	1.00	29.68
297	CG	ARG	A	35	58.842	47.176	19.053	1.00	33.37
300	CD	ARG	A	35	59.681	46.648	17.895	1.00	36.27
303	NE	ARG	A	35	59.113	45.445	17.291	1.00	39.06
305	CZ	ARG	A	35	59.778	44.630	16.473	1.00	41.04
306	NH1	ARG	A	35	61.046	44.878	16.153	1.00	42.52
309	NH2	ARG	A	35	59.174	43.564	15.970	1.00	42.39
312	C	ARG	A	35	59.426	49.761	21.828	1.00	28.40
313	O	ARG	A	35	59.480	49.210	22.926	1.00	27.74
314	N	PHE	A	36	60.045	50.910	21.557	1.00	27.61
316	CA	PHE	A	36	60.785	51.634	22.587	1.00	27.39
318	CB	PHE	A	36	61.853	52.533	21.960	1.00	27.18
321	CG	PHE	A	36	62.924	51.766	21.240	1.00	25.69
322	CD1	PHE	A	36	63.214	52.029	19.918	1.00	25.01
324	CE1	PHE	A	36	64.194	51.311	19.253	1.00	25.43
326	CZ	PHE	A	36	64.881	50.295	19.910	1.00	26.41
328	CE2	PHE	A	36	64.600	50.022	21.218	1.00	26.08
330	CD2	PHE	A	36	63.624	50.755	21.886	1.00	25.98
332	C	PHE	A	36	59.855	52.427	23.491	1.00	27.72
333	O	PHE	A	36	60.189	52.684	24.642	1.00	27.44
334	N	ILE	A	37	58.679	52.775	22.979	1.00	27.76
336	CA	ILE	A	37	57.677	53.488	23.756	1.00	28.44
338	CB	ILE	A	37	56.779	54.342	22.815	1.00	28.50
340	CG1	ILE	A	37	57.527	55.620	22.419	1.00	28.68
343	CD1	ILE	A	37	56.932	56.377	21.266	1.00	29.67
347	CG2	ILE	A	37	55.440	54.687	23.473	1.00	29.47
351	C	ILE	A	37	56.831	52.526	24.620	1.00	28.85
352	O	ILE	A	37	56.394	52.900	25.707	1.00	29.06
353	N	ALA	A	38	56.631	51.293	24.156	1.00	29.01
355	CA	ALA	A	38	55.688	50.357	24.797	1.00	29.51
357	CB	ALA	A	38	55.489	49.108	23.926	1.00	29.54
361	C	ALA	A	38	55.995	49.951	26.251	1.00	29.76
362	O	ALA	A	38	55.058	49.805	27.032	1.00	30.41
363	N	PRO	A	39	57.261	49.761	26.631	1.00	29.96
364	CA	PRO	A	39	57.590	49.430	28.028	1.00	29.81
366	CB	PRO	A	39	59.019	48.871	27.952	1.00	29.63
369	CG	PRO	A	39	59.465	48.986	26.511	1.00	30.25
372	CD	PRO	A	39	58.466	49.813	25.784	1.00	30.23
375	C	PRO	A	39	57.547	50.605	29.003	1.00	29.35
376	O	PRO	A	39	57.768	50.409	30.200	1.00	29.40
377	N	LEU	A	40	57.288	51.808	28.508	1.00	28.66
379	CA	LEU	A	40	57.243	52.978	29.364	1.00	27.78
381	CB	LEU	A	40	57.200	54.260	28.535	1.00	27.92
384	CG	LEU	A	40	58.410	54.574	27.654	1.00	28.42
386	CD1	LEU	A	40	58.185	55.906	26.946	1.00	29.06
390	CD2	LEU	A	40	59.716	54.573	28.481	1.00	28.93
394	C	LEU	A	40	56.009	52.911	30.243	1.00	27.39
395	O	LEU	A	40	54.962	52.410	29.814	1.00	27.10
396	N	PRO	A	41	56.115	53.412	31.471	1.00	26.65
397	CA	PRO	A	41	54.937	53.506	32.338	1.00	26.24
399	CB	PRO	A	41	55.528	53.818	33.719	1.00	26.42

FIGURE 3 (Cont.)AE

A	B	C	D	E	F	G	H	I	J
402	CG	PRO	A	41	56.887	54.444	33.440	1.00	26.56
405	CD	PRO	A	41	57.339	53.909	32.122	1.00	26.41
408	C	PRO	A	41	54.017	54.624	31.863	1.00	25.76
409	O	PRO	A	41	54.386	55.397	30.977	1.00	25.20
410	N	PHE	A	42	52.840	54.706	32.469	1.00	25.70
412	CA	PHE	A	42	51.873	55.765	32.212	1.00	25.79
414	CB	PHE	A	42	52.479	57.131	32.556	1.00	25.87
417	CG	PHE	A	42	53.188	57.147	33.878	1.00	25.55
418	CD1	PHE	A	42	52.489	56.876	35.049	1.00	25.97
420	CE1	PHE	A	42	53.131	56.864	36.274	1.00	25.51
422	CZ	PHE	A	42	54.480	57.116	36.349	1.00	25.34
424	CE2	PHE	A	42	55.195	57.379	35.186	1.00	25.76
426	CD2	PHE	A	42	54.551	57.383	33.959	1.00	24.78
428	C	PHE	A	42	51.323	55.730	30.787	1.00	25.98
429	O	PHE	A	42	50.987	56.762	30.226	1.00	25.18
430	N	GLN	A	43	51.222	54.528	30.221	1.00	26.46
432	CA	GLN	A	43	50.537	54.330	28.942	1.00	27.47
434	CB	GLN	A	43	50.502	52.854	28.527	1.00	27.56
437	CG	GLN	A	43	51.828	52.229	28.185	1.00	28.72
440	CD	GLN	A	43	52.596	52.968	27.106	1.00	30.09
441	OE1	GLN	A	43	53.817	53.065	27.187	1.00	32.82
442	NE2	GLN	A	43	51.897	53.475	26.096	1.00	30.99
445	C	GLN	A	43	49.111	54.786	29.106	1.00	28.28
446	O	GLN	A	43	48.511	54.598	30.172	1.00	28.52
447	N	ASN	A	44	48.579	55.403	28.060	1.00	28.97
449	CA	ASN	A	44	47.202	55.868	28.040	1.00	29.76
451	CB	ASN	A	44	46.212	54.687	28.180	1.00	30.31
454	CG	ASN	A	44	46.513	53.535	27.210	1.00	31.66
455	OD1	ASN	A	44	46.576	53.726	25.997	1.00	36.40
456	ND2	ASN	A	44	46.694	52.342	27.748	1.00	32.76
459	C	ASN	A	44	46.937	56.948	29.094	1.00	29.56
460	O	ASN	A	44	45.842	57.041	29.631	1.00	29.84
461	N	THR	A	45	47.958	57.750	29.393	1.00	29.02
463	CA	THR	A	45	47.782	59.023	30.090	1.00	28.55
465	CB	THR	A	45	48.663	59.090	31.346	1.00	28.99
467	OG1	THR	A	45	50.045	59.094	30.966	1.00	29.70
469	CG2	THR	A	45	48.504	57.836	32.213	1.00	29.52
473	C	THR	A	45	48.173	60.135	29.107	1.00	27.72
474	O	THR	A	45	48.886	59.861	28.147	1.00	27.59
475	N	PRO	A	46	47.713	61.371	29.316	1.00	26.46
476	CA	PRO	A	46	47.961	62.453	28.351	1.00	25.93
478	CB	PRO	A	46	47.404	63.699	29.061	1.00	25.92
481	CG	PRO	A	46	46.331	63.155	29.974	1.00	26.20
484	CD	PRO	A	46	46.879	61.831	30.447	1.00	26.74
487	C	PRO	A	46	49.419	62.688	27.918	1.00	25.28
488	O	PRO	A	46	49.638	62.912	26.731	1.00	24.82
489	N	VAL	A	47	50.389	62.661	28.824	1.00	24.84
491	CA	VAL	A	47	51.766	62.944	28.412	1.00	24.49
493	CB	VAL	A	47	52.711	63.189	29.616	1.00	24.35
495	CG1	VAL	A	47	52.934	61.920	30.414	1.00	25.47
499	CG2	VAL	A	47	54.047	63.752	29.131	1.00	25.13
503	C	VAL	A	47	52.317	61.860	27.460	1.00	23.84

FIGURE 3 ~~(Cont.)~~ AF

A	B	C	D	E	F	G	H	I	J
504	O	VAL	A	47	52.962	62.172	26.462	1.00	23.42
505	N	VAL	A	48	52.046	60.594	27.752	1.00	23.38
507	CA	VAL	A	48	52.505	59.516	26.878	1.00	23.48
509	CB	VAL	A	48	52.449	58.146	27.567	1.00	23.07
511	CG1	VAL	A	48	52.773	57.012	26.566	1.00	23.03
515	CG2	VAL	A	48	53.409	58.125	28.740	1.00	23.55
519	C	VAL	A	48	51.725	59.512	25.567	1.00	23.67
520	O	VAL	A	48	52.297	59.299	24.510	1.00	23.73
521	N	GLU	A	49	50.427	59.782	25.632	1.00	23.99
523	CA	GLU	A	49	49.629	59.897	24.417	1.00	24.17
525	CB	GLU	A	49	48.155	60.087	24.761	1.00	24.86
528	CG	GLU	A	49	47.534	58.863	25.404	1.00	27.67
531	CD	GLU	A	49	46.125	59.115	25.899	1.00	33.01
532	OE1	GLU	A	49	45.337	58.140	25.909	1.00	36.58
533	OE2	GLU	A	49	45.806	60.274	26.278	1.00	35.89
534	C	GLU	A	49	50.115	61.066	23.562	1.00	22.99
535	O	GLU	A	49	50.099	60.980	22.345	1.00	21.91
536	N	THR	A	50	50.574	62.139	24.208	1.00	22.14
538	CA	THR	A	50	51.147	63.270	23.497	1.00	21.71
540	CB	THR	A	50	51.426	64.447	24.442	1.00	21.87
542	OG1	THR	A	50	50.218	64.833	25.112	1.00	21.63
544	CG2	THR	A	50	51.861	65.695	23.647	1.00	21.55
548	C	THR	A	50	52.435	62.833	22.813	1.00	21.19
549	O	THR	A	50	52.658	63.152	21.667	1.00	20.77
550	N	MET	A	51	53.268	62.075	23.515	1.00	21.45
552	CA	MET	A	51	54.525	61.583	22.936	1.00	21.16
554	CB	MET	A	51	55.321	60.768	23.965	1.00	21.28
557	CG	MET	A	51	55.825	61.558	25.165	1.00	21.06
560	SD	MET	A	51	56.503	60.485	26.448	1.00	21.92
561	CE	MET	A	51	58.036	59.941	25.581	1.00	18.94
565	C	MET	A	51	54.227	60.713	21.704	1.00	21.05
566	O	MET	A	51	54.873	60.858	20.676	1.00	21.01
567	N	GLN	A	52	53.228	59.835	21.812	1.00	21.04
569	CA	GLN	A	52	.52.882	58.908	20.737	1.00	21.29
571	CB	GLN	A	52	51.862	57.889	21.229	1.00	21.77
574	CG	GLN	A	52	52.407	56.822	22.155	1.00	23.17
577	CD	GLN	A	52	51.297	55.954	22.728	1.00	26.61
578	OE1	GLN	A	52	51.254	54.743	22.480	1.00	30.25
579	NE2	GLN	A	52	50.389	56.569	23.474	1.00	24.83
582	C	GLN	A	52	52.299	59.642	19.526	1.00	21.06
583	O	GLN	A	52	52.547	59.291	18.371	1.00	19.85
584	N	TYR	A	53	51.495	60.656	19.804	1.00	20.82
586	CA	TYR	A	53	50.887	61.466	18.760	1.00	21.28
588	CB	TYR	A	53	49.946	62.447	19.433	1.00	21.43
591	CG	TYR	A	53	49.135	63.357	18.555	1.00	23.00
592	CD1	TYR	A	53	47.838	63.002	18.154	1.00	24.56
594	CE1	TYR	A	53	47.069	63.859	17.385	1.00	24.49
596	CZ	TYR	A	53	47.562	65.107	17.052	1.00	25.48
597	OH	TYR	A	53	46.793	65.965	16.292	1.00	24.53
599	CE2	TYR	A	53	48.844	65.484	17.445	1.00	23.07
601	CD2	TYR	A	53	49.604	64.618	18.212	1.00	23.55
603	C	TYR	A	53	51.967	62.218	18.002	1.00	20.79

FIGURE 3 (Cont.)AG

A	B	C	D	E	F	G	H	I	J
604	O	TYR	A	53	52.033	62.184	16.765	1.00	20.35
605	N	GLY	A	54	52.811	62.910	18.761	1.00	20.69
607	CA	GLY	A	54	53.840	63.751	18.187	1.00	20.90
610	C	GLY	A	54	54.963	62.972	17.526	1.00	21.30
611	O	GLY	A	54	55.596	63.495	16.627	1.00	21.54
612	N	ALA	A	55	55.215	61.732	17.955	1.00	21.95
614	CA	ALA	A	55	56.315	60.942	17.389	1.00	22.16
616	CB	ALA	A	55	56.981	60.100	18.480	1.00	22.04
620	C	ALA	A	55	55.862	60.033	16.242	1.00	22.84
621	O	ALA	A	55	56.609	59.808	15.282	1.00	22.77
622	N	LEU	A	56	54.645	59.506	16.337	1.00	23.82
624	CA	LEU	A	56	54.227	58.413	15.446	1.00	25.01
626	CB	LEU	A	56	53.718	57.229	16.272	1.00	25.40
629	CG	LEU	A	56	54.803	56.448	16.999	1.00	26.02
631	CD1	LEU	A	56	54.192	55.617	18.110	1.00	27.58
635	CD2	LEU	A	56	55.583	55.570	16.011	1.00	26.63
639	C	LEU	A	56	53.188	58.758	14.386	1.00	25.71
640	O	LEU	A	56	53.144	58.088	13.352	1.00	25.79
641	N	LEU	A	57	52.351	59.772	14.626	1.00	26.23
643	CA	LEU	A	57	51.244	60.076	13.712	1.00	26.84
645	CB	LEU	A	57	50.045	60.627	14.487	1.00	27.25
648	CG	LEU	A	57	48.675	60.380	13.836	1.00	29.61
650	CD1	LEU	A	57	48.417	58.886	13.617	1.00	30.97
654	CD2	LEU	A	57	47.544	60.990	14.672	1.00	31.15
658	C	LEU	A	57	51.660	61.041	12.589	1.00	26.56
659	O	LEU	A	57	51.650	62.260	12.762	1.00	26.92
660	N	GLY	A	58	52.014	60.471	11.441	1.00	26.04
662	CA	GLY	A	58	52.480	61.230	10.294	1.00	25.24
665	C	GLY	A	58	53.983	61.421	10.347	1.00	24.44
666	O	GLY	A	58	54.635	61.015	11.301	1.00	24.64
667	N	GLY	A	59	54.513	62.081	9.331	1.00	23.73
669	CA	GLY	A	59	55.938	62.322	9.195	1.00	23.06
672	C	GLY	A	59	56.553	61.359	8.209	1.00	22.26
673	O	GLY	A	59	56.162	60.194	8.133	1.00	22.42
674	N	LYS	A	60	57.547	61.842	7.478	1.00	22.13
676	CA	LYS	A	60	58.154	61.112	6.374	1.00	21.99
678	CB	LYS	A	60	58.759	62.101	5.373	1.00	22.38
681	CG	LYS	A	60	57.740	63.053	4.741	1.00	22.42
684	CD	LYS	A	60	58.397	63.946	3.700	1.00	22.36
687	CE	LYS	A	60	59.309	65.000	4.315	1.00	22.65
690	NZ	LYS	A	60	58.610	65.764	5.390	1.00	22.32
694	C	LYS	A	60	59.236	60.121	6.820	1.00	21.22
695	O	LYS	A	60	59.639	59.250	6.044	1.00	21.45
696	N	ARG	A	61	59.679	60.268	8.064	1.00	20.48
698	CA	ARG	A	61	60.763	59.494	8.657	1.00	19.82
700	CB	ARG	A	61	60.347	58.035	8.877	1.00	19.66
703	CG	ARG	A	61	59.138	57.855	9.723	1.00	20.10
706	CD	ARG	A	61	59.272	58.230	11.192	1.00	20.40
709	NE	ARG	A	61	57.948	58.049	11.781	1.00	20.92
711	CZ	ARG	A	61	57.037	58.991	11.934	1.00	22.13
712	NH1	ARG	A	61	57.298	60.255	11.645	1.00	23.06
715	NH2	ARG	A	61	55.840	58.667	12.421	1.00	22.86

FIGURE 3 (Cont.)AH

A	B	C	D	E	F	G	H	I	J
718	C	ARG	A	61	62.061	59.514	7.860	1.00	19.24
719	O	ARG	A	61	62.738	58.501	7.779	1.00	18.48
720	N	LEU	A	62	62.432	60.666	7.307	1.00	18.87
722	CA	LEU	A	62	63.630	60.734	6.485	1.00	18.40
724	CB	LEU	A	62	63.643	61.988	5.629	1.00	18.86
727	CG	LEU	A	62	62.430	62.083	4.708	1.00	18.30
729	CD1	LEU	A	62	62.550	63.320	3.821	1.00	18.04
733	CD2	LEU	A	62	62.266	60.815	3.896	1.00	19.13
737	C	LEU	A	62	64.908	60.646	7.296	1.00	18.46
738	O	LEU	A	62	65.933	60.241	6.772	1.00	18.88
739	N	ARG	A	63	64.866	61.017	8.562	1.00	17.65
741	CA	ARG	A	63	66.054	60.871	9.384	1.00	17.87
743	CB	ARG	A	63	66.000	61.756	10.611	1.00	17.85
746	CG	ARG	A	63	66.045	63.219	10.223	1.00	17.38
749	CD	ARG	A	63	65.459	64.177	11.253	1.00	17.84
752	NE	ARG	A	63	65.361	65.533	10.704	1.00	19.01
754	CZ	ARG	A	63	64.417	65.941	9.863	1.00	20.05
755	NH1	ARG	A	63	64.422	67.193	9.411	1.00	22.90
758	NH2	ARG	A	63	63.449	65.123	9.477	1.00	21.09
761	C	ARG	A	63	66.322	59.401	9.705	1.00	17.71
762	O	ARG	A	63	67.454	58.951	9.531	1.00	18.10
763	N	PRO	A	64	65.329	58.645	10.163	1.00	17.51
764	CA	PRO	A	64	65.476	57.180	10.192	1.00	17.45
766	CB	PRO	A	64	64.070	56.703	10.531	1.00	17.56
769	CG	PRO	A	64	63.506	57.791	11.356	1.00	17.73
772	CD	PRO	A	64	64.052	59.064	10.767	1.00	17.18
775	C	PRO	A	64	65.936	56.615	8.859	1.00	17.33
776	O	PRO	A	64	66.816	55.755	8.854	1.00	17.25
777	N	PHE	A	65	65.376	57.104	7.754	1.00	17.93
779	CA	PHE	A	65	65.781	56.677	6.427	1.00	18.40
781	CB	PHE	A	65	65.044	57.457	5.338	1.00	19.10
784	CG	PHE	A	65	65.198	56.872	3.941	1.00	19.82
785	CD1	PHE	A	65	66.425	56.898	3.278	1.00	21.48
787	CE1	PHE	A	65	66.558	56.356	1.990	1.00	24.16
789	CZ	PHE	A	65	65.456	55.801	1.354	1.00	23.70
791	CE2	PHE	A	65	64.232	55.787	2.000	1.00	24.40
793	CD2	PHE	A	65	64.112	56.329	3.289	1.00	21.85
795	C	PHE	A	65	67.288	56.831	6.274	1.00	18.39
796	O	PHE	A	65	67.951	55.920	5.814	1.00	18.40
797	N	LEU	A	66	67.820	57.973	6.683	1.00	18.52
799	CA	LEU	A	66	69.255	58.228	6.643	1.00	18.77
801	CB	LEU	A	66	69.554	59.650	7.101	1.00	19.16
804	CG	LEU	A	66	69.280	60.737	6.070	1.00	20.56
806	CD1	LEU	A	66	69.409	62.108	6.739	1.00	21.70
810	CD2	LEU	A	66	70.233	60.611	4.897	1.00	21.14
814	C	LEU	A	66	70.063	57.274	7.512	1.00	18.22
815	O	LEU	A	66	71.162	56.862	7.131	1.00	17.84
816	N	VAL	A	67	69.546	56.973	8.693	1.00	16.88
818	CA	VAL	A	67	70.235	56.066	9.609	1.00	17.06
820	CB	VAL	A	67	69.512	56.001	10.969	1.00	16.98
822	CG1	VAL	A	67	70.075	54.909	11.865	1.00	17.14
826	CG2	VAL	A	67	69.621	57.337	11.679	1.00	16.69

FIGURE 3 (Cont.)AI

A	B	C	D	E	F	G	H	I	J
830	C	VAL	A	67	70.315	54.667	8.984	1.00	17.43
831	O	VAL	A	67	71.391	54.087	8.924	1.00	16.85
832	N	TYR	A	68	69.171	54.175	8.504	1.00	17.82
834	CA	TYR	A	68	69.049	52.853	7.890	1.00	18.73
836	CB	TYR	A	68	67.590	52.546	7.534	1.00	18.65
839	CG	TYR	A	68	66.682	52.294	8.706	1.00	17.77
840	CD1	TYR	A	68	66.993	51.343	9.670	1.00	18.53
842	CE1	TYR	A	68	66.152	51.109	10.734	1.00	19.24
844	CZ	TYR	A	68	64.967	51.819	10.844	1.00	17.86
845	OH	TYR	A	68	64.123	51.616	11.915	1.00	16.87
847	CE2	TYR	A	68	64.650	52.774	9.914	1.00	18.34
849	CD2	TYR	A	68	65.492	52.988	8.835	1.00	18.14
851	C	TYR	A	68	69.878	52.741	6.626	1.00	19.22
852	O	TYR	A	68	70.627	51.788	6.466	1.00	20.65
853	N	ALA	A	69	69.762	53.725	5.744	1.00	19.41
855	CA	ALA	A	69	70.470	53.707	4.474	1.00	19.53
857	CB	ALA	A	69	70.035	54.875	3.616	1.00	20.02
861	C	ALA	A	69	71.975	53.744	4.695	1.00	20.18
862	O	ALA	A	69	72.721	53.053	4.011	1.00	21.39
863	N	THR	A	70	72.423	54.545	5.656	1.00	20.00
865	CA	THR	A	70	73.841	54.656	5.930	1.00	20.26
867	CB	THR	A	70	74.124	55.842	6.828	1.00	20.06
869	OG1	THR	A	70	73.742	57.060	6.143	1.00	19.95
871	CG2	THR	A	70	75.624	55.979	7.077	1.00	20.73
875	C	THR	A	70	74.371	53.370	6.527	1.00	20.27
876	O	THR	A	70	75.330	52.821	6.025	1.00	20.97
877	N	GLY	A	71	73.743	52.886	7.588	1.00	20.36
879	CA	GLY	A	71	74.136	51.630	8.199	1.00	20.44
882	C	GLY	A	71	74.090	50.470	7.229	1.00	20.43
883	O	GLY	A	71	74.966	49.600	7.242	1.00	21.38
884	N	HIS	A	72	73.061	50.442	6.393	1.00	21.26
886	CA	HIS	A	72	72.886	49.367	5.401	1.00	21.95
888	CB	HIS	A	72	71.577	49.530	4.623	1.00	22.16
891	CG	HIS	A	72	70.369	49.049	5.362	1.00	21.95
892	ND1	HIS	A	72	69.094	49.468	5.051	1.00	23.29
894	CE1	HIS	A	72	68.231	48.892	5.869	1.00	23.63
896	NE2	HIS	A	72	68.899	48.097	6.687	1.00	21.16
898	CD2	HIS	A	72	70.238	48.181	6.394	1.00	22.72
900	C	HIS	A	72	74.054	49.313	4.421	1.00	22.56
901	O	HIS	A	72	74.455	48.228	3.995	1.00	21.64
902	N	MET	A	73	74.610	50.477	4.080	1.00	23.05
904	CA	MET	A	73	75.782	50.536	3.201	1.00	23.89
906	CB	MET	A	73	76.282	51.961	3.027	1.00	24.12
909	CG	MET	A	73	75.546	52.765	2.016	1.00	26.38
912	SD	MET	A	73	76.590	54.090	1.347	1.00	31.06
913	CE	MET	A	73	77.179	54.849	2.837	1.00	30.61
917	C	MET	A	73	76.944	49.713	3.732	1.00	24.04
918	O	MET	A	73	77.740	49.208	2.945	1.00	24.70
919	N	PHE	A	74	77.052	49.617	5.057	1.00	24.12
921	CA	PHE	A	74	78.122	48.863	5.723	1.00	24.15
923	CB	PHE	A	74	78.644	49.693	6.881	1.00	24.28
926	CG	PHE	A	74	79.127	51.040	6.455	1.00	25.09

FIGURE 3 (Cont.)AJ

A	B	C	D	E	F	G	H	I	J
927	CD1	PHE	A	74	78.410	52.183	6.759	1.00	25.88
929	CE1	PHE	A	74	78.847	53.424	6.357	1.00	25.67
931	CZ	PHE	A	74	80.015	53.547	5.641	1.00	26.11
933	CE2	PHE	A	74	80.751	52.415	5.330	1.00	26.51
935	CD2	PHE	A	74	80.305	51.167	5.736	1.00	26.10
937	C	PHE	A	74	77.710	47.461	6.196	1.00	24.09
938	O	PHE	A	74	78.475	46.770	6.875	1.00	23.88
939	N	GLY	A	75	76.508	47.039	5.815	1.00	23.45
941	CA	GLY	A	75	76.025	45.708	6.114	1.00	23.38
944	C	GLY	A	75	75.544	45.539	7.545	1.00	23.11
945	O	GLY	A	75	75.412	44.415	8.032	1.00	22.14
946	N	VAL	A	76	75.261	46.636	8.241	1.00	22.50
948	CA	VAL	A	76	74.698	46.461	9.577	1.00	22.69
950	CB	VAL	A	76	75.093	47.576	10.642	1.00	22.92
952	CG1	VAL	A	76	75.915	48.711	10.067	1.00	23.76
956	CG2	VAL	A	76	73.908	48.074	11.396	1.00	22.71
960	C	VAL	A	76	73.194	46.144	9.484	1.00	21.96
961	O	VAL	A	76	72.487	46.604	8.591	1.00	21.42
962	N	SER	A	77	72.746	45.302	10.402	1.00	21.48
964	CA	SER	A	77	71.389	44.778	10.405	1.00	21.77
966	CB	SER	A	77	71.250	43.671	11.467	1.00	22.01
969	OG	SER	A	77	69.901	43.269	11.656	1.00	24.55
971	C	SER	A	77	70.388	45.893	10.669	1.00	21.66
972	O	SER	A	77	70.614	46.768	11.497	1.00	20.52
973	N	THR	A	78	69.280	45.849	9.950	1.00	21.30
975	CA	THR	A	78	68.197	46.782	10.145	1.00	21.37
977	CB	THR	A	78	67.041	46.395	9.243	1.00	21.59
979	OG1	THR	A	78	67.522	46.238	7.898	1.00	20.65
981	CG2	THR	A	78	66.004	47.531	9.175	1.00	21.88
985	C	THR	A	78	67.742	46.839	11.609	1.00	21.40
986	O	THR	A	78	67.457	47.919	12.127	1.00	20.26
987	N	ASN	A	79	67.712	45.681	12.273	1.00	20.85
989	CA	ASN	A	79	67.259	45.592	13.665	1.00	21.11
991	CB	ASN	A	79	67.155	44.113	14.110	1.00	20.78
994	CG	ASN	A	79	66.777	43.962	15.577	1.00	20.57
995	OD1	ASN	A	79	65.629	44.176	15.960	1.00	20.74
996	ND2	ASN	A	79	67.741	43.572	16.395	1.00	21.96
999	C	ASN	A	79	68.135	46.366	14.648	1.00	21.18
1000	O	ASN	A	79	67.630	46.935	15.589	1.00	21.24
1001	N	THR	A	80	69.445	46.363	14.445	1.00	21.31
1003	CA	THR	A	80	70.325	47.176	15.288	1.00	22.18
1005	CB	THR	A	80	71.831	46.719	15.233	1.00	23.07
1007	OG1	THR	A	80	72.729	47.845	15.254	1.00	25.14
1009	CG2	THR	A	80	72.163	46.051	13.972	1.00	25.36
1013	C	THR	A	80	70.149	48.653	14.952	1.00	21.28
1014	O	THR	A	80	70.191	49.488	15.836	1.00	21.18
1015	N	LEU	A	81	69.889	48.958	13.685	1.00	20.13
1017	CA	LEU	A	81	69.699	50.338	13.267	1.00	19.67
1019	CB	LEU	A	81	69.773	50.458	11.743	1.00	19.03
1022	CG	LEU	A	81	71.174	50.220	11.203	1.00	20.05
1024	CD1	LEU	A	81	71.133	49.777	9.747	1.00	20.55
1028	CD2	LEU	A	81	72.025	51.477	11.362	1.00	21.66

FIGURE 3 (Cont.)AK

A	B	C	D	E	F	G	H	I	J
1032	C	LEU	A	81	68.395	50.943	13.785	1.00	19.10
1033	O	LEU	A	81	68.266	52.154	13.797	1.00	17.73
1034	N	ASP	A	82	67.452	50.098	14.213	1.00	18.92
1036	CA	ASP	A	82	66.206	50.555	14.808	1.00	19.26
1038	CB	ASP	A	82	65.374	49.380	15.347	1.00	19.80
1041	CG	ASP	A	82	64.537	48.689	14.279	1.00	21.07
1042	OD1	ASP	A	82	64.370	49.232	13.167	1.00	22.88
1043	OD2	ASP	A	82	63.977	47.584	14.496	1.00	22.05
1044	C	ASP	A	82	66.491	51.503	15.972	1.00	18.72
1045	O	ASP	A	82	65.743	52.455	16.193	1.00	18.90
1046	N	ALA	A	83	67.551	51.227	16.724	1.00	18.47
1048	CA	ALA	A	83	67.879	52.031	17.902	1.00	18.05
1050	CB	ALA	A	83	68.957	51.350	18.777	1.00	18.08
1054	C	ALA	A	83	68.262	53.464	17.528	1.00	17.75
1055	O	ALA	A	83	67.571	54.391	17.954	1.00	16.58
1056	N	PRO	A	84	69.334	53.674	16.754	1.00	17.46
1057	CA	PRO	A	84	69.660	55.034	16.310	1.00	17.24
1059	CB	PRO	A	84	70.978	54.870	15.537	1.00	17.48
1062	CG	PRO	A	84	71.073	53.397	15.176	1.00	17.90
1065	CD	PRO	A	84	70.318	52.690	16.274	1.00	17.39
1068	C	PRO	A	84	68.570	55.674	15.452	1.00	17.54
1069	O	PRO	A	84	68.372	56.871	15.546	1.00	16.99
1070	N	ALA	A	85	67.881	54.899	14.617	1.00	17.55
1072	CA	ALA	A	85	66.786	55.439	13.827	1.00	17.51
1074	CB	ALA	A	85	66.196	54.371	12.908	1.00	17.15
1078	C	ALA	A	85	65.710	56.010	14.751	1.00	17.33
1079	O	ALA	A	85	65.235	57.120	14.540	1.00	17.48
1080	N	ALA	A	86	65.365	55.276	15.797	1.00	17.28
1082	CA	ALA	A	86	64.309	55.702	16.702	1.00	17.98
1084	CB	ALA	A	86	63.858	54.558	17.575	1.00	17.95
1088	C	ALA	A	86	64.764	56.881	17.559	1.00	18.07
1089	O	ALA	A	86	63.986	57.800	17.828	1.00	18.55
1090	N	ALA	A	87	66.027	56.852	17.965	1.00	17.63
1092	CA	ALA	A	87	66.612	57.905	18.776	1.00	17.90
1094	CB	ALA	A	87	68.016	57.551	19.129	1.00	17.89
1098	C	ALA	A	87	66.602	59.238	18.046	1.00	18.01
1099	O	ALA	A	87	66.199	60.258	18.611	1.00	16.96
1100	N	VAL	A	88	67.076	59.233	16.802	1.00	18.36
1102	CA	VAL	A	88	67.108	60.469	16.022	1.00	19.02
1104	CB	VAL	A	88	67.919	60.359	14.706	1.00	19.48
1106	CG1	VAL	A	88	69.346	59.943	15.004	1.00	21.38
1110	CG2	VAL	A	88	67.262	59.431	13.694	1.00	20.88
1114	C	VAL	A	88	65.697	60.984	15.728	1.00	18.91
1115	O	VAL	A	88	65.478	62.192	15.694	1.00	19.41
1116	N	GLU	A	89	64.755	60.075	15.506	1.00	18.77
1118	CA	GLU	A	89	63.371	60.460	15.281	1.00	19.03
1120	CB	GLU	A	89	62.580	59.307	14.672	1.00	19.35
1123	CG	GLU	A	89	61.202	59.659	14.140	1.00	20.47
1126	CD	GLU	A	89	61.187	60.686	13.014	1.00	23.08
1127	OE1	GLU	A	89	60.085	61.188	12.699	1.00	21.79
1128	OE2	GLU	A	89	62.243	61.001	12.436	1.00	22.95
1129	C	GLU	A	89	62.726	60.972	16.571	1.00	19.06

FIGURE 3 ~~(Cont.)~~AL

A	B	C	D	E	F	G	H	I	J
1130	O	GLU	A	89	61.883	61.856	16.515	1.00	18.98
1131	N	CYS	A	90	63.154	60.466	17.724	1.00	19.07
1133	CA	CYS	A	90	62.684	61.026	18.999	1.00	19.48
1135	CB	CYS	A	90	63.154	60.218	20.204	1.00	19.62
1138	SG	CYS	A	90	62.240	58.692	20.462	1.00	21.40
1139	C	CYS	A	90	63.139	62.464	19.144	1.00	18.83
1140	O	CYS	A	90	62.348	63.311	19.526	1.00	19.11
1141	N	ILE	A	91	64.405	62.740	18.846	1.00	18.13
1143	CA	ILE	A	91	64.900	64.108	18.934	1.00	17.94
1145	CB	ILE	A	91	66.402	64.201	18.602	1.00	18.00
1147	CG1	ILE	A	91	67.269	63.442	19.628	1.00	18.23
1150	CD1	ILE	A	91	67.160	63.942	21.057	1.00	18.91
1154	CG2	ILE	A	91	66.824	65.659	18.520	1.00	18.94
1158	C	ILE	A	91	64.117	64.994	17.959	1.00	17.15
1159	O	ILE	A	91	63.700	66.094	18.308	1.00	16.79
1160	N	HIS	A	92	63.952	64.506	16.732	1.00	16.32
1162	CA	HIS	A	92	63.238	65.238	15.701	1.00	16.58
1164	CB	HIS	A	92	63.182	64.438	14.409	1.00	16.65
1167	CG	HIS	A	92	62.424	65.119	13.321	1.00	16.27
1168	ND1	HIS	A	92	61.352	64.536	12.675	1.00	17.53
1170	CE1	HIS	A	92	60.892	65.378	11.761	1.00	15.88
1172	NE2	HIS	A	92	61.620	66.480	11.800	1.00	17.29
1174	CD2	HIS	A	92	62.573	66.348	12.779	1.00	15.01
1176	C	HIS	A	92	61.825	65.555	16.167	1.00	16.53
1177	O	HIS	A	92	61.399	66.712	16.151	1.00	16.57
1178	N	ALA	A	93	61.119	64.532	16.620	1.00	15.86
1180	CA	ALA	A	93	59.753	64.699	17.119	1.00	16.23
1182	CB	ALA	A	93	59.177	63.346	17.566	1.00	16.25
1186	C	ALA	A	93	59.671	65.720	18.251	1.00	16.36
1187	O	ALA	A	93	58.753	66.544	18.297	1.00	16.22
1188	N	TYR	A	94	60.632	65.668	19.168	1.00	16.81
1190	CA	TYR	A	94	60.653	66.585	20.289	1.00	17.25
1192	CB	TYR	A	94	61.742	66.187	21.312	1.00	18.09
1195	CG	TYR	A	94	62.785	67.233	21.639	1.00	18.65
1196	CD1	TYR	A	94	62.444	68.391	22.309	1.00	20.51
1198	CE1	TYR	A	94	63.388	69.341	22.613	1.00	22.48
1200	CZ	TYR	A	94	64.701	69.138	22.248	1.00	22.20
1201	OH	TYR	A	94	65.628	70.083	22.565	1.00	24.51
1203	CE2	TYR	A	94	65.075	67.983	21.590	1.00	21.60
1205	CD2	TYR	A	94	64.122	67.037	21.306	1.00	19.95
1207	C	TYR	A	94	60.837	68.001	19.766	1.00	17.28
1208	O	TYR	A	94	60.178	68.921	20.232	1.00	16.91
1209	N	SER	A	95	61.709	68.169	18.780	1.00	17.12
1211	CA	SER	A	95	62.028	69.486	18.281	1.00	17.61
1213	CB	SER	A	95	63.209	69.446	17.312	1.00	17.91
1216	OG	SER	A	95	62.859	68.946	16.045	1.00	19.03
1218	C	SER	A	95	60.787	70.161	17.665	1.00	18.18
1219	O	SER	A	95	60.591	71.367	17.826	1.00	17.08
1220	N	LEU	A	96	59.936	69.376	17.021	1.00	18.08
1222	CA	LEU	A	96	58.748	69.937	16.356	1.00	18.75
1224	CB	LEU	A	96	58.168	68.946	15.359	1.00	18.81
1227	CG	LEU	A	96	59.159	68.371	14.350	1.00	19.61

FIGURE 3 (Cont.)AM

A	B	C	D	E	F	G	H	I	J
1229	CD1	LEU	A	96	58.421	67.472	13.385	1.00	19.87
1233	CD2	LEU	A	96	59.901	69.477	13.628	1.00	20.82
1237	C	LEU	A	96	57.676	70.285	17.371	1.00	18.79
1238	O	LEU	A	96	56.928	71.252	17.192	1.00	19.67
1239	N	ILE	A	97	57.581	69.478	18.422	1.00	18.80
1241	CA	ILE	A	97	56.574	69.704	19.448	1.00	18.69
1243	CB	ILE	A	97	56.590	68.612	20.520	1.00	18.23
1245	CG1	ILE	A	97	56.062	67.307	19.941	1.00	17.66
1248	CD1	ILE	A	97	56.017	66.149	20.924	1.00	19.38
1252	CG2	ILE	A	97	55.756	69.050	21.746	1.00	18.51
1256	C	ILE	A	97	56.844	71.069	20.071	1.00	19.44
1257	O	ILE	A	97	55.925	71.851	20.233	1.00	19.55
1258	N	HIS	A	98	58.108	71.358	20.383	1.00	19.42
1260	CA	HIS	A	98	58.452	72.609	21.039	1.00	20.66
1262	CB	HIS	A	98	59.797	72.507	21.730	1.00	21.50
1265	CG	HIS	A	98	59.735	71.795	23.045	1.00	25.90
1266	ND1	HIS	A	98	59.610	70.432	23.149	1.00	34.19
1268	CE1	HIS	A	98	59.570	70.087	24.425	1.00	32.41
1270	NE2	HIS	A	98	59.660	71.175	25.149	1.00	32.34
1272	CD2	HIS	A	98	59.748	72.261	24.312	1.00	32.88
1274	C	HIS	A	98	58.437	73.774	20.072	1.00	20.22
1275	O	HIS	A	98	58.095	74.880	20.444	1.00	20.04
1276	N	ASP	A	99	58.809	73.500	18.829	1.00	20.34
1278	CA	ASP	A	99	58.834	74.488	17.772	1.00	20.27
1280	CB	ASP	A	99	59.394	73.845	16.496	1.00	20.14
1283	CG	ASP	A	99	59.438	74.806	15.326	1.00	19.89
1284	OD1	ASP	A	99	58.542	74.720	14.458	1.00	20.18
1285	OD2	ASP	A	99	60.332	75.665	15.194	1.00	18.02
1286	C	ASP	A	99	57.447	75.081	17.512	1.00	20.91
1287	O	ASP	A	99	57.322	76.277	17.253	1.00	21.26
1288	N	ASP	A	100	56.410	74.254	17.580	1.00	21.41
1290	CA	ASP	A	100	55.037	74.718	17.328	1.00	21.41
1292	CB	ASP	A	100	54.098	73.551	17.048	1.00	21.45
1295	CG	ASP	A	100	54.436	72.819	15.799	1.00	20.29
1296	OD1	ASP	A	100	54.167	71.594	15.734	1.00	20.18
1297	OD2	ASP	A	100	54.978	73.379	14.841	1.00	19.29
1298	C	ASP	A	100	54.428	75.500	18.483	1.00	21.71
1299	O	ASP	A	100	53.395	76.123	18.301	1.00	22.06
1300	N	LEU	A	101	55.039	75.467	19.664	1.00	21.73
1302	CA	LEU	A	101	54.463	76.129	20.837	1.00	21.71
1304	CB	LEU	A	101	55.389	76.027	22.052	1.00	21.29
1307	CG	LEU	A	101	55.643	74.639	22.631	1.00	21.02
1309	CD1	LEU	A	101	56.681	74.748	23.744	1.00	21.63
1313	CD2	LEU	A	101	54.375	73.987	23.130	1.00	21.37
1317	C	LEU	A	101	54.173	77.611	20.587	1.00	22.13
1318	O	LEU	A	101	54.852	78.255	19.795	1.00	21.48
1319	N	PRO	A	102	53.167	78.152	21.273	1.00	23.19
1320	CA	PRO	A	102	52.850	79.588	21.175	1.00	23.59
1322	CB	PRO	A	102	51.811	79.779	22.282	1.00	24.00
1325	CG	PRO	A	102	51.099	78.464	22.308	1.00	23.90
1328	CD	PRO	A	102	52.216	77.443	22.149	1.00	22.62
1331	C	PRO	A	102	54.045	80.533	21.348	1.00	24.21

FIGURE 3 ~~(Cont.)~~AN

A	B	C	D	E	F	G	H	I	J
1332	O	PRO	A	102	54.148	81.494	20.599	1.00	25.11
1333	N	ALA	A	103	54.943	80.255	22.285	1.00	24.74
1335	CA	ALA	A	103	56.123	81.094	22.516	1.00	25.23
1337	CB	ALA	A	103	56.753	80.737	23.867	1.00	25.78
1341	C	ALA	A	103	57.176	80.941	21.417	1.00	25.46
1342	O	ALA	A	103	58.093	81.742	21.317	1.00	24.70
1343	N	MET	A	104	57.053	79.879	20.626	1.00	25.19
1345	CA	MET	A	104	57.981	79.590	19.550	1.00	26.00
1347	CB	MET	A	104	58.362	78.109	19.598	1.00	25.79
1350	CG	MET	A	104	58.997	77.719	20.916	1.00	27.52
1353	SD	MET	A	104	60.690	78.194	20.987	1.00	31.55
1354	CE	MET	A	104	61.411	77.093	19.688	1.00	31.97
1358	C	MET	A	104	57.345	79.995	18.207	1.00	25.73
1359	O	MET	A	104	57.213	81.186	17.942	1.00	25.54
1360	N	ASP	A	105	56.937	79.038	17.374	1.00	25.29
1362	CA	ASP	A	105	56.373	79.388	16.061	1.00	25.81
1364	CB	ASP	A	105	56.832	78.419	14.969	1.00	25.24
1367	CG	ASP	A	105	58.319	78.496	14.716	1.00	24.83
1368	OD1	ASP	A	105	58.853	77.642	13.954	1.00	22.09
1369	OD2	ASP	A	105	59.049	79.364	15.253	1.00	25.62
1370	C	ASP	A	105	54.851	79.525	16.069	1.00	25.92
1371	O	ASP	A	105	54.289	80.054	15.126	1.00	26.07
1372	N	ASP	A	106	54.206	79.043	17.125	1.00	26.89
1374	CA	ASP	A	106	52.759	79.211	17.350	1.00	27.69
1376	CB	ASP	A	106	52.419	80.670	17.671	1.00	28.12
1379	CG	ASP	A	106	51.000	80.840	18.202	1.00	29.63
1380	OD1	ASP	A	106	50.458	81.960	18.094	1.00	31.75
1381	OD2	ASP	A	106	50.342	79.911	18.732	1.00	31.76
1382	C	ASP	A	106	51.952	78.715	16.157	1.00	28.05
1383	O	ASP	A	106	51.159	79.450	15.549	1.00	28.01
1384	N	ASP	A	107	52.190	77.456	15.809	1.00	28.07
1386	CA	ASP	A	107	51.534	76.822	14.686	1.00	27.99
1388	CB	ASP	A	107	52.553	76.037	13.855	1.00	28.56
1391	CG	ASP	A	107	53.069	76.830	12.677	1.00	29.78
1392	OD1	ASP	A	107	52.257	77.111	11.774	1.00	33.36
1393	OD2	ASP	A	107	54.255	77.210	12.549	1.00	31.90
1394	C	ASP	A	107	50.478	75.882	15.230	1.00	27.64
1395	O	ASP	A	107	50.693	75.218	16.248	1.00	26.98
1396	N	ASP	A	108	49.334	75.823	14.559	1.00	26.95
1398	CA	ASP	A	108	48.242	74.989	15.031	1.00	26.81
1400	CB	ASP	A	108	46.929	75.778	15.089	1.00	27.66
1403	CG	ASP	A	108	46.453	76.241	13.725	1.00	30.37
1404	OD1	ASP	A	108	45.282	76.700	13.645	1.00	33.61
1405	OD2	ASP	A	108	47.165	76.194	12.690	1.00	32.04
1406	C	ASP	A	108	48.075	73.702	14.236	1.00	25.96
1407	O	ASP	A	108	47.283	72.856	14.631	1.00	25.76
1408	N	LEU	A	109	48.818	73.559	13.136	1.00	25.04
1410	CA	LEU	A	109	48.751	72.367	12.298	1.00	24.85
1412	CB	LEU	A	109	48.106	72.694	10.945	1.00	25.33
1415	CG	LEU	A	109	46.598	72.821	10.810	1.00	26.83
1417	CD1	LEU	A	109	46.260	73.283	9.399	1.00	29.44
1421	CD2	LEU	A	109	45.903	71.492	11.089	1.00	27.95

FIGURE 3 ~~(Cont.)~~ AO

A	B	C	D	E	F	G	H	I	J
1425	C	LEU	A	109	50.144	71.781	12.034	1.00	23.64
1426	O	LEU	A	109	51.094	72.514	11.790	1.00	23.64
1427	N	ARG	A	110	50.237	70.454	12.081	1.00	22.79
1429	CA	ARG	A	110	51.401	69.715	11.603	1.00	22.20
1431	CB	ARG	A	110	52.479	69.644	12.672	1.00	21.90
1434	CG	ARG	A	110	53.742	69.015	12.166	1.00	21.62
1437	CD	ARG	A	110	54.820	68.975	13.195	1.00	21.16
1440	NE	ARG	A	110	55.377	70.290	13.472	1.00	19.55
1442	CZ	ARG	A	110	56.277	70.905	12.721	1.00	21.19
1443	NH1	ARG	A	110	56.740	72.082	13.111	1.00	21.55
1446	NH2	ARG	A	110	56.737	70.355	11.590	1.00	21.98
1449	C	ARG	A	110	50.997	68.301	11.215	1.00	21.87
1450	O	ARG	A	110	50.184	67.686	11.876	1.00	20.97
1451	N	ARG	A	111	51.566	67.807	10.122	1.00	22.79
1453	CA	ARG	A	111	51.237	66.489	9.580	1.00	23.42
1455	CB	ARG	A	111	51.814	65.407	10.477	1.00	23.33
1458	CG	ARG	A	111	53.310	65.424	10.531	1.00	22.10
1461	CD	ARG	A	111	53.841	64.752	11.768	1.00	21.59
1464	NE	ARG	A	111	55.282	64.632	11.726	1.00	21.10
1466	CZ	ARG	A	111	56.009	64.082	12.681	1.00	21.03
1467	NH1	ARG	A	111	55.438	63.576	13.760	1.00	20.75
1470	NH2	ARG	A	111	57.323	64.020	12.544	1.00	22.79
1473	C	ARG	A	111	49.733	66.284	9.374	1.00	24.49
1474	O	ARG	A	111	49.216	65.181	9.528	1.00	24.90
1475	N	GLY	A	112	49.048	67.375	9.037	1.00	25.84
1477	CA	GLY	A	112	47.641	67.363	8.673	1.00	26.45
1480	C	GLY	A	112	46.709	67.432	9.854	1.00	27.01
1481	O	GLY	A	112	45.500	67.383	9.663	1.00	27.66
1482	N	LEU	A	113	47.258	67.574	11.066	1.00	27.18
1484	CA	LEU	A	113	46.478	67.445	12.301	1.00	27.29
1486	CB	LEU	A	113	46.778	66.104	12.965	1.00	27.61
1489	CG	LEU	A	113	46.308	64.849	12.230	1.00	29.25
1491	CD1	LEU	A	113	46.956	63.639	12.826	1.00	29.40
1495	CD2	LEU	A	113	44.799	64.723	12.297	1.00	30.33
1499	C	LEU	A	113	46.783	68.580	13.279	1.00	26.95
1500	O	LEU	A	113	47.781	69.273	13.134	1.00	26.97
1501	N	PRO	A	114	45.911	68.807	14.256	1.00	26.77
1502	CA	PRO	A	114	46.242	69.737	15.341	1.00	26.42
1504	CB	PRO	A	114	45.151	69.465	16.391	1.00	26.39
1507	CG	PRO	A	114	43.997	68.927	15.636	1.00	27.10
1510	CD	PRO	A	114	44.540	68.278	14.377	1.00	27.03
1513	C	PRO	A	114	47.644	69.428	15.902	1.00	25.96
1514	O	PRO	A	114	47.988	68.247	16.088	1.00	25.12
1515	N	THR	A	115	48.433	70.470	16.131	1.00	25.63
1517	CA	THR	A	115	49.730	70.336	16.803	1.00	25.53
1519	CB	THR	A	115	50.478	71.668	16.835	1.00	25.67
1521	OG1	THR	A	115	49.605	72.715	17.288	1.00	26.41
1523	CG2	THR	A	115	50.901	72.085	15.442	1.00	25.77
1527	C	THR	A	115	49.531	69.838	18.228	1.00	25.27
1528	O	THR	A	115	48.430	69.941	18.787	1.00	24.78
1529	N	CYS	A	116	50.600	69.305	18.817	1.00	24.89
1531	CA	CYS	A	116	50.523	68.697	20.137	1.00	24.95

FIGURE 3 (Cont.)AP

A	B	C	D	E	F	G	H	I	J
1533	CB	CYS	A	116	51.895	68.165	20.581	1.00	24.90
1536	SG	CYS	A	116	52.285	66.565	19.821	1.00	24.91
1537	C	CYS	A	116	49.933	69.634	21.182	1.00	24.97
1538	O	CYS	A	116	49.096	69.228	21.971	1.00	24.71
1539	N	HIS	A	117	50.346	70.894	21.168	1.00	25.78
1541	CA	HIS	A	117	49.925	71.820	22.208	1.00	26.16
1543	CB	HIS	A	117	50.836	73.054	22.246	1.00	26.51
1546	CG	HIS	A	117	50.548	74.067	21.186	1.00	27.10
1547	ND1	HIS	A	117	50.785	73.840	19.849	1.00	30.89
1549	CE1	HIS	A	117	50.441	74.911	19.156	1.00	30.52
1551	NE2	HIS	A	117	50.007	75.831	19.996	1.00	30.35
1553	CD2	HIS	A	117	50.066	75.327	21.272	1.00	29.44
1555	C	HIS	A	117	48.433	72.162	22.054	1.00	26.69
1556	O	HIS	A	117	47.747	72.385	23.040	1.00	26.52
1557	N	VAL	A	118	47.938	72.180	20.820	1.00	27.17
1559	CA	VAL	A	118	46.510	72.380	20.577	1.00	27.86
1561	CB	VAL	A	118	46.217	72.617	19.078	1.00	27.70
1563	CG1	VAL	A	118	44.701	72.510	18.774	1.00	28.86
1567	CG2	VAL	A	118	46.737	73.972	18.645	1.00	28.14
1571	C	VAL	A	118	45.695	71.196	21.131	1.00	28.24
1572	O	VAL	A	118	44.784	71.396	21.935	1.00	28.47
1573	N	LYS	A	119	46.040	69.973	20.733	1.00	28.54
1575	CA	LYS	A	119	45.245	68.798	21.101	1.00	29.34
1577	CB	LYS	A	119	45.617	67.583	20.241	1.00	29.61
1580	CG	LYS	A	119	44.863	66.301	20.626	1.00	30.82
1583	CD	LYS	A	119	45.106	65.186	19.627	1.00	32.53
1586	CE	LYS	A	119	44.199	63.976	19.839	1.00	33.76
1589	NZ	LYS	A	119	43.344	64.050	21.054	1.00	36.05
1593	C	LYS	A	119	45.371	68.422	22.581	1.00	29.59
1594	O	LYS	A	119	44.383	68.012	23.194	1.00	29.82
1595	N	PHE	A	120	46.575	68.551	23.146	1.00	28.84
1597	CA	PHE	A	120	46.839	68.108	24.519	1.00	28.62
1599	CB	PHE	A	120	47.984	67.096	24.529	1.00	28.31
1602	CG	PHE	A	120	47.722	65.880	23.711	1.00	27.28
1603	CD1	PHE	A	120	47.055	64.787	24.261	1.00	27.38
1605	CE1	PHE	A	120	46.831	63.631	23.508	1.00	27.16
1607	CZ	PHE	A	120	47.271	63.563	22.198	1.00	27.58
1609	CE2	PHE	A	120	47.932	64.648	21.636	1.00	27.23
1611	CD2	PHE	A	120	48.163	65.804	22.399	1.00	27.44
1613	C	PHE	A	120	47.185	69.217	25.515	1.00	28.26
1614	O	PHE	A	120	47.341	68.943	26.706	1.00	29.25
1615	N	GLY	A	121	47.299	70.452	25.042	1.00	27.60
1617	CA	GLY	A	121	47.659	71.575	25.896	1.00	26.94
1620	C	GLY	A	121	49.155	71.840	25.860	1.00	26.46
1621	O	GLY	A	121	49.958	70.992	25.438	1.00	26.06
1622	N	GLU	A	122	49.536	73.009	26.340	1.00	25.72
1624	CA	GLU	A	122	50.910	73.462	26.248	1.00	25.58
1626	CB	GLU	A	122	51.007	74.958	26.519	1.00	25.87
1629	CG	GLU	A	122	50.483	75.783	25.358	1.00	29.11
1632	CD	GLU	A	122	50.355	77.241	25.698	1.00	33.26
1633	OE1	GLU	A	122	51.247	77.754	26.399	1.00	35.51
1634	OE2	GLU	A	122	49.349	77.861	25.269	1.00	37.97

FIGURE 3 ~~(Cont.)~~ AQ

A	B	C	D	E	F	G	H	I	J
1635	C	GLU	A	122	51.798	72.689	27.211	1.00	24.80
1636	O	GLU	A	122	52.899	72.300	26.840	1.00	24.40
1637	N	ALA	A	123	51.320	72.474	28.436	1.00	23.77
1639	CA	ALA	A	123	52.098	71.760	29.447	1.00	23.73
1641	CB	ALA	A	123	51.353	71.711	30.776	1.00	23.98
1645	C	ALA	A	123	52.441	70.343	28.968	1.00	23.81
1646	O	ALA	A	123	53.603	69.943	29.024	1.00	24.19
1647	N	ASN	A	124	51.442	69.609	28.479	1.00	22.86
1649	CA	ASN	A	124	51.654	68.270	27.947	1.00	22.86
1651	CB	ASN	A	124	50.345	67.623	27.491	1.00	23.02
1654	CG	ASN	A	124	49.539	67.041	28.635	1.00	24.68
1655	OD1	ASN	A	124	48.304	67.110	28.640	1.00	27.85
1656	ND2	ASN	A	124	50.220	66.461	29.600	1.00	25.67
1659	C	ASN	A	124	52.631	68.261	26.779	1.00	21.84
1660	O	ASN	A	124	53.428	67.339	26.667	1.00	22.15
1661	N	ALA	A	125	52.543	69.263	25.908	1.00	20.33
1663	CA	ALA	A	125	53.457	69.399	24.788	1.00	20.39
1665	CB	ALA	A	125	52.984	70.529	23.886	1.00	20.63
1669	C	ALA	A	125	54.925	69.621	25.250	1.00	19.95
1670	O	ALA	A	125	55.856	68.974	24.760	1.00	19.97
1671	N	ILE	A	126	55.117	70.509	26.218	1.00	19.41
1673	CA	ILE	A	126	56.434	70.769	26.790	1.00	19.39
1675	CB	ILE	A	126	56.357	71.842	27.880	1.00	19.07
1677	CG1	ILE	A	126	56.032	73.214	27.267	1.00	20.58
1680	CD1	ILE	A	126	55.450	74.180	28.244	1.00	22.11
1684	CG2	ILE	A	126	57.668	71.944	28.623	1.00	19.77
1688	C	ILE	A	126	57.011	69.487	27.378	1.00	19.19
1689	O	ILE	A	126	58.134	69.105	27.069	1.00	18.97
1690	N	LEU	A	127	56.229	68.824	28.211	1.00	18.52
1692	CA	LEU	A	127	56.694	67.637	28.913	1.00	19.19
1694	CB	LEU	A	127	55.716	67.252	30.029	1.00	19.06
1697	CG	LEU	A	127	55.616	68.280	31.166	1.00	20.37
1699	CD1	LEU	A	127	56.961	68.500	31.859	1.00	22.60
1703	CD2	LEU	A	127	54.595	67.820	32.159	1.00	21.48
1707	C	LEU	A	127	56.907	66.470	27.966	1.00	18.53
1708	O	LEU	A	127	57.856	65.723	28.126	1.00	18.41
1709	N	ALA	A	128	56.033	66.320	26.973	1.00	17.92
1711	CA	ALA	A	128	56.179	65.228	26.012	1.00	17.62
1713	CB	ALA	A	128	54.947	65.115	25.104	1.00	17.67
1717	C	ALA	A	128	57.434	65.418	25.168	1.00	17.09
1718	O	ALA	A	128	58.108	64.461	24.828	1.00	17.12
1719	N	GLY	A	129	57.740	66.649	24.807	1.00	16.81
1721	CA	GLY	A	129	58.945	66.914	24.059	1.00	16.96
1724	C	GLY	A	129	60.155	66.651	24.946	1.00	17.30
1725	O	GLY	A	129	61.102	66.022	24.500	1.00	17.59
1726	N	ASP	A	130	60.106	67.121	26.193	1.00	17.16
1728	CA	ASP	A	130	61.139	66.853	27.190	1.00	17.77
1730	CB	ASP	A	130	60.717	67.383	28.562	1.00	18.20
1733	CG	ASP	A	130	60.801	68.881	28.661	1.00	19.18
1734	OD1	ASP	A	130	61.407	69.492	27.759	1.00	21.99
1735	OD2	ASP	A	130	60.295	69.527	29.612	1.00	19.91
1736	C	ASP	A	130	61.410	65.359	27.301	1.00	17.64

FIGURE 3 (Cont.)AR

A	B	C	D	E	F	G	H	I	J
1737	O	ASP	A	130	62.548	64.927	27.230	1.00	17.90
1738	N	ALA	A	131	60.343	64.584	27.447	1.00	17.42
1740	CA	ALA	A	131	60.438	63.146	27.633	1.00	17.39
1742	CB	ALA	A	131	59.098	62.582	28.089	1.00	17.97
1746	C	ALA	A	131	60.910	62.429	26.378	1.00	17.06
1747	O	ALA	A	131	61.576	61.425	26.482	1.00	16.51
1748	N	LEU	A	132	60.525	62.918	25.197	1.00	17.23
1750	CA	LEU	A	132	61.005	62.333	23.947	1.00	17.60
1752	CB	LEU	A	132	60.265	62.904	22.740	1.00	17.59
1755	CG	LEU	A	132	58.930	62.247	22.427	1.00	17.08
1757	CD1	LEU	A	132	58.170	63.044	21.399	1.00	18.87
1761	CD2	LEU	A	132	59.126	60.798	21.970	1.00	18.78
1765	C	LEU	A	132	62.515	62.534	23.779	1.00	17.74
1766	O	LEU	A	132	63.197	61.641	23.297	1.00	17.61
1767	N	GLN	A	133	63.036	63.695	24.185	1.00	17.96
1769	CA	GLN	A	133	64.483	63.926	24.148	1.00	18.23
1771	CB	GLN	A	133	64.894	65.366	24.559	1.00	18.28
1774	CG	GLN	A	133	66.427	65.512	24.520	1.00	19.50
1777	CD	GLN	A	133	67.021	66.816	25.074	1.00	22.38
1778	OE1	GLN	A	133	66.350	67.833	25.237	1.00	19.65
1779	NE2	GLN	A	133	68.322	66.768	25.346	1.00	23.26
1782	C	GLN	A	133	65.165	62.906	25.043	1.00	17.62
1783	O	GLN	A	133	66.132	62.284	24.645	1.00	17.06
1784	N	THR	A	134	64.650	62.736	26.258	1.00	18.05
1786	CA	THR	A	134	65.220	61.790	27.201	1.00	18.07
1788	CB	THR	A	134	64.461	61.797	28.520	1.00	18.89
1790	OG1	THR	A	134	64.445	63.109	29.073	1.00	17.91
1792	CG2	THR	A	134	65.189	60.940	29.551	1.00	18.65
1796	C	THR	A	134	65.165	60.373	26.665	1.00	17.74
1797	O	THR	A	134	66.111	59.615	26.829	1.00	17.70
1798	N	LEU	A	135	64.056	60.037	26.016	1.00	17.32
1800	CA	LEU	A	135	63.863	58.698	25.487	1.00	17.21
1802	CB	LEU	A	135	62.450	58.554	24.899	1.00	16.68
1805	CG	LEU	A	135	62.102	57.160	24.360	1.00	17.14
1807	CD1	LEU	A	135	62.252	56.096	25.413	1.00	17.24
1811	CD2	LEU	A	135	60.691	57.141	23.772	1.00	17.71
1815	C	LEU	A	135	64.934	58.362	24.443	1.00	16.99
1816	O	LEU	A	135	65.396	57.234	24.373	1.00	17.51
1817	N	ALA	A	136	65.311	59.345	23.637	1.00	16.86
1819	CA	ALA	A	136	66.350	59.191	22.640	1.00	16.98
1821	CB	ALA	A	136	66.617	60.525	21.936	1.00	16.96
1825	C	ALA	A	136	67.629	58.656	23.286	1.00	17.44
1826	O	ALA	A	136	68.269	57.772	22.741	1.00	17.77
1827	N	PHE	A	137	67.982	59.193	24.449	1.00	17.78
1829	CA	PHE	A	137	69.179	58.770	25.172	1.00	18.09
1831	CB	PHE	A	137	69.700	59.891	26.062	1.00	18.06
1834	CG	PHE	A	137	70.113	61.073	25.279	1.00	18.66
1835	CD1	PHE	A	137	69.308	62.203	25.215	1.00	17.95
1837	CE1	PHE	A	137	69.672	63.284	24.422	1.00	18.78
1839	CZ	PHE	A	137	70.834	63.241	23.689	1.00	18.81
1841	CE2	PHE	A	137	71.647	62.108	23.742	1.00	19.03
1843	CD2	PHE	A	137	71.277	61.031	24.526	1.00	19.55

FIGURE 3 ~~(Cont.)~~AS

A	B	C	D	E	F	G	H	I	J
1845	C	PHE	A	137	69.000	57.481	25.944	1.00	17.78
1846	O	PHE	A	137	69.967	56.741	26.093	1.00	19.01
1847	N	SER	A	138	67.783	57.181	26.383	1.00	17.63
1849	CA	SER	A	138	67.480	55.853	26.930	1.00	17.81
1851	CB	SER	A	138	66.064	55.790	27.503	1.00	18.14
1854	OG	SER	A	138	65.998	56.474	28.749	1.00	19.62
1856	C	SER	A	138	67.634	54.788	25.860	1.00	17.61
1857	O	SER	A	138	68.139	53.706	26.127	1.00	17.31
1858	N	ILE	A	139	67.202	55.100	24.646	1.00	17.34
1860	CA	ILE	A	139	67.275	54.150	23.545	1.00	18.07
1862	CB	ILE	A	139	66.528	54.676	22.286	1.00	18.17
1864	CG1	ILE	A	139	65.001	54.638	22.531	1.00	18.76
1867	CD1	ILE	A	139	64.188	55.429	21.499	1.00	19.79
1871	CG2	ILE	A	139	66.878	53.836	21.073	1.00	19.10
1875	C	ILE	A	139	68.732	53.827	23.237	1.00	17.54
1876	O	ILE	A	139	69.102	52.663	23.207	1.00	17.29
1877	N	LEU	A	140	69.556	54.854	23.081	1.00	17.52
1879	CA	LEU	A	140	70.961	54.677	22.710	1.00	18.26
1881	CB	LEU	A	140	71.607	56.028	22.388	1.00	18.48
1884	CG	LEU	A	140	71.151	56.649	21.066	1.00	18.76
1886	CD1	LEU	A	140	71.890	57.952	20.786	1.00	19.92
1890	CD2	LEU	A	140	71.349	55.663	19.939	1.00	19.54
1894	C	LEU	A	140	71.775	53.986	23.786	1.00	18.96
1895	O	LEU	A	140	72.715	53.265	23.476	1.00	18.14
1896	N	SER	A	141	71.414	54.201	25.046	1.00	19.45
1898	CA	SER	A	141	72.165	53.596	26.142	1.00	20.52
1900	CB	SER	A	141	72.125	54.482	27.404	1.00	20.39
1903	OG	SER	A	141	70.812	54.763	27.813	1.00	22.72
1905	C	SER	A	141	71.707	52.157	26.439	1.00	20.99
1906	O	SER	A	141	72.535	51.344	26.874	1.00	21.12
1907	N	ASP	A	142	70.435	51.840	26.157	1.00	20.94
1909	CA	ASP	A	142	69.803	50.583	26.617	1.00	21.52
1911	CB	ASP	A	142	68.510	50.885	27.360	1.00	21.35
1914	CG	ASP	A	142	68.740	51.573	28.668	1.00	23.16
1915	OD1	ASP	A	142	67.745	52.038	29.261	1.00	22.75
1916	OD2	ASP	A	142	69.871	51.678	29.188	1.00	24.41
1917	C	ASP	A	142	69.436	49.569	25.557	1.00	21.65
1918	O	ASP	A	142	69.308	48.382	25.850	1.00	20.45
1919	N	ALA	A	143	69.203	50.033	24.342	1.00	22.42
1921	CA	ALA	A	143	68.645	49.176	23.301	1.00	23.31
1923	CB	ALA	A	143	68.113	50.004	22.165	1.00	22.74
1927	C	ALA	A	143	69.698	48.200	22.795	1.00	24.09
1928	O	ALA	A	143	70.895	48.453	22.888	1.00	24.03
1929	N	ASP	A	144	69.228	47.087	22.256	1.00	25.84
1931	CA	ASP	A	144	70.096	46.051	21.707	1.00	27.11
1933	CB	ASP	A	144	69.309	44.768	21.402	1.00	27.68
1936	CG	ASP	A	144	68.293	44.426	22.469	1.00	31.56
1937	OD1	ASP	A	144	67.116	44.829	22.309	1.00	38.25
1938	OD2	ASP	A	144	68.558	43.752	23.487	1.00	35.92
1939	C	ASP	A	144	70.716	46.563	20.420	1.00	26.94
1940	O	ASP	A	144	69.995	46.966	19.504	1.00	27.42
1941	N	MET	A	145	72.044	46.586	20.374	1.00	27.00

FIGURE 3 (Cont.)AT

A	B	C	D	E	F	G	H	I	J
1943	CA	MET	A	145	72.794	46.828	19.148	1.00	27.40
1945	CB	MET	A	145	73.297	48.273	19.105	1.00	27.32
1948	CG	MET	A	145	72.199	49.301	19.048	1.00	27.17
1951	SD	MET	A	145	72.806	50.970	18.731	1.00	27.97
1952	CE	MET	A	145	73.747	51.294	20.169	1.00	26.35
1956	C	MET	A	145	73.972	45.850	19.125	1.00	28.08
1957	O	MET	A	145	75.099	46.213	19.487	1.00	27.86
1958	N	PRO	A	146	73.702	44.596	18.768	1.00	28.99
1959	CA	PRO	A	146	74.700	43.519	18.900	1.00	29.80
1961	CB	PRO	A	146	74.018	42.301	18.244	1.00	30.17
1964	CG	PRO	A	146	72.730	42.788	17.654	1.00	29.78
1967	CD	PRO	A	146	72.402	44.090	18.296	1.00	29.22
1970	C	PRO	A	146	76.088	43.778	18.280	1.00	29.90
1971	O	PRO	A	146	77.081	43.394	18.874	1.00	30.77
1972	N	GLU	A	147	76.176	44.452	17.149	1.00	30.07
1974	CA	GLU	A	147	77.488	44.605	16.495	1.00	30.29
1976	CB	GLU	A	147	77.348	44.666	14.970	1.00	30.88
1979	CG	GLU	A	147	76.419	43.625	14.368	1.00	33.60
1982	CD	GLU	A	147	74.996	44.126	14.226	1.00	36.03
1983	OE1	GLU	A	147	74.447	44.088	13.102	1.00	38.00
1984	OE2	GLU	A	147	74.433	44.556	15.252	1.00	37.12
1985	C	GLU	A	147	78.224	45.857	16.976	1.00	28.68
1986	O	GLU	A	147	79.335	46.129	16.528	1.00	28.50
1987	N	VAL	A	148	77.599	46.613	17.879	1.00	26.68
1989	CA	VAL	A	148	78.056	47.949	18.205	1.00	25.01
1991	CB	VAL	A	148	76.886	48.966	18.244	1.00	25.12
1993	CG1	VAL	A	148	77.404	50.369	18.438	1.00	24.25
1997	CG2	VAL	A	148	76.049	48.887	16.950	1.00	24.80
2001	C	VAL	A	148	78.819	47.927	19.526	1.00	23.84
2002	O	VAL	A	148	78.271	47.605	20.585	1.00	23.11
2003	N	SER	A	149	80.098	48.254	19.440	1.00	22.76
2005	CA	SER	A	149	80.952	48.338	20.613	1.00	22.78
2007	CB	SER	A	149	82.404	48.597	20.186	1.00	22.49
2010	OG	SER	A	149	82.568	49.915	19.707	1.00	21.57
2012	C	SER	A	149	80.458	49.448	21.539	1.00	23.11
2013	O	SER	A	149	79.794	50.402	21.099	1.00	21.95
2014	N	ASP	A	150	80.777	49.313	22.817	1.00	23.66
2016	CA	ASP	A	150	80.499	50.348	23.801	1.00	24.49
2018	CB	ASP	A	150	81.010	49.930	25.172	1.00	25.14
2021	CG	ASP	A	150	80.256	48.733	25.735	1.00	27.65
2022	OD1	ASP	A	150	80.719	48.186	26.762	1.00	31.30
2023	OD2	ASP	A	150	79.201	48.281	25.225	1.00	27.89
2024	C	ASP	A	150	81.115	51.680	23.394	1.00	24.45
2025	O	ASP	A	150	80.499	52.725	23.568	1.00	23.41
2026	N	ARG	A	151	82.319	51.639	22.827	1.00	24.28
2028	CA	ARG	A	151	82.973	52.844	22.355	1.00	24.79
2030	CB	ARG	A	151	84.352	52.508	21.759	1.00	26.00
2033	CG	ARG	A	151	85.134	53.699	21.268	1.00	28.93
2036	CD	ARG	A	151	85.432	54.712	22.350	1.00	34.80
2039	NE	ARG	A	151	84.576	55.893	22.233	1.00	38.89
2041	CZ	ARG	A	151	84.277	56.711	23.229	1.00	42.07
2042	NH1	ARG	A	151	83.494	57.756	22.989	1.00	43.97

FIGURE 3 ~~(Cont.)~~AU

A	B	C	D	E	F	G	H	I	J
2045	NH2	ARG	A	151	84.754	56.502	24.462	1.00	42.69
2048	C	ARG	A	151	82.119	53.534	21.303	1.00	23.63
2049	O	ARG	A	151	81.949	54.749	21.330	1.00	22.68
2050	N	ASP	A	152	81.578	52.751	20.377	1.00	22.64
2052	CA	ASP	A	152	80.765	53.305	19.316	1.00	22.05
2054	CB	ASP	A	152	80.695	52.351	18.126	1.00	22.68
2057	CG	ASP	A	152	82.013	52.303	17.348	1.00	24.58
2058	OD1	ASP	A	152	82.780	53.285	17.412	1.00	24.51
2059	OD2	ASP	A	152	82.369	51.328	16.654	1.00	27.53
2060	C	ASP	A	152	79.380	53.730	19.832	1.00	20.89
2061	O	ASP	A	152	78.829	54.703	19.348	1.00	19.41
2062	N	ARG	A	153	78.855	53.043	20.844	1.00	19.83
2064	CA	ARG	A	153	77.577	53.435	21.459	1.00	18.66
2066	CB	ARG	A	153	77.116	52.390	22.450	1.00	18.96
2069	CG	ARG	A	153	75.734	52.644	23.008	1.00	18.87
2072	CD	ARG	A	153	75.377	51.687	24.112	1.00	19.73
2075	NE	ARG	A	153	75.180	50.322	23.630	1.00	20.07
2077	CZ	ARG	A	153	73.991	49.773	23.369	1.00	22.06
2078	NH1	ARG	A	153	73.929	48.516	22.949	1.00	20.83
2081	NH2	ARG	A	153	72.862	50.466	23.521	1.00	23.23
2084	C	ARG	A	153	77.724	54.771	22.171	1.00	18.18
2085	O	ARG	A	153	76.842	55.612	22.081	1.00	17.20
2086	N	ILE	A	154	78.847	54.959	22.869	1.00	17.73
2088	CA	ILE	A	154	79.141	56.223	23.542	1.00	18.41
2090	CB	ILE	A	154	80.414	56.100	24.449	1.00	18.14
2092	CG1	ILE	A	154	80.092	55.249	25.684	1.00	19.24
2095	CD1	ILE	A	154	81.307	54.703	26.408	1.00	20.01
2099	CG2	ILE	A	154	80.932	57.468	24.875	1.00	19.53
2103	C	ILE	A	154	79.277	57.343	22.505	1.00	17.74
2104	O	ILE	A	154	78.757	58.424	22.698	1.00	18.17
2105	N	SER	A	155	79.934	57.063	21.388	1.00	18.18
2107	CA	SER	A	155	80.095	58.043	20.323	1.00	18.52
2109	CB	SER	A	155	81.020	57.511	19.236	1.00	18.63
2112	OG	SER	A	155	82.330	57.395	19.748	1.00	18.50
2114	C	SER	A	155	78.744	58.437	19.718	1.00	19.05
2115	O	SER	A	155	78.538	59.594	19.368	1.00	19.13
2116	N	MET	A	156	77.836	57.476	19.618	1.00	19.12
2118	CA	MET	A	156	76.482	57.743	19.135	1.00	19.40
2120	CB	MET	A	156	75.674	56.461	19.063	1.00	19.56
2123	CG	MET	A	156	76.083	55.564	17.948	1.00	22.23
2126	SD	MET	A	156	74.922	54.182	17.803	1.00	28.16
2127	CE	MET	A	156	75.814	53.241	16.666	1.00	26.77
2131	C	MET	A	156	75.746	58.693	20.039	1.00	18.61
2132	O	MET	A	156	75.101	59.609	19.567	1.00	18.79
2133	N	ILE	A	157	75.826	58.439	21.342	1.00	18.55
2135	CA	ILE	A	157	75.194	59.281	22.349	1.00	17.91
2137	CB	ILE	A	157	75.342	58.649	23.752	1.00	17.84
2139	CG1	ILE	A	157	74.511	57.360	23.840	1.00	18.27
2142	CD1	ILE	A	157	74.814	56.495	25.017	1.00	18.88
2146	CG2	ILE	A	157	74.941	59.646	24.845	1.00	17.97
2150	C	ILE	A	157	75.804	60.685	22.313	1.00	17.61
2151	O	ILE	A	157	75.087	61.683	22.308	1.00	16.93

FIGURE 3 (Cont.)AV

A	B	C	D	E	F	G	H	I	J
2152	N	SER	A	158	77.136	60.749	22.290	1.00	17.36
2154	CA	SER	A	158	77.856	62.012	22.247	1.00	17.24
2156	CB	SER	A	158	79.372	61.759	22.292	1.00	17.57
2159	OG	SER	A	158	80.087	62.908	21.936	1.00	16.92
2161	C	SER	A	158	77.487	62.819	21.007	1.00	17.58
2162	O	SER	A	158	77.266	64.003	21.093	1.00	17.17
2163	N	GLU	A	159	77.408	62.163	19.856	1.00	18.38
2165	CA	GLU	A	159	77.042	62.833	18.616	1.00	18.63
2167	CB	GLU	A	159	77.242	61.904	17.409	1.00	19.18
2170	CG	GLU	A	159	76.518	62.361	16.145	1.00	20.77
2173	CD	GLU	A	159	76.979	63.726	15.666	1.00	23.75
2174	OE1	GLU	A	159	78.105	64.141	16.022	1.00	24.45
2175	OE2	GLU	A	159	76.233	64.384	14.918	1.00	26.52
2176	C	GLU	A	159	75.592	63.324	18.648	1.00	18.90
2177	O	GLU	A	159	75.311	64.455	18.224	1.00	18.41
2178	N	LEU	A	160	74.671	62.489	19.122	1.00	18.15
2180	CA	LEU	A	160	73.274	62.921	19.169	1.00	18.98
2182	CB	LEU	A	160	72.333	61.801	19.559	1.00	19.20
2185	CG	LEU	A	160	70.845	62.123	19.337	1.00	20.03
2187	CD1	LEU	A	160	70.528	62.479	17.890	1.00	20.04
2191	CD2	LEU	A	160	70.015	60.977	19.795	1.00	21.02
2195	C	LEU	A	160	73.119	64.115	20.113	1.00	19.39
2196	O	LEU	A	160	72.388	65.058	19.808	1.00	19.39
2197	N	ALA	A	161	73.832	64.078	21.234	1.00	19.92
2199	CA	ALA	A	161	73.814	65.162	22.208	1.00	20.54
2201	CB	ALA	A	161	74.591	64.764	23.463	1.00	20.76
2205	C	ALA	A	161	74.362	66.466	21.621	1.00	20.84
2206	O	ALA	A	161	73.690	67.496	21.678	1.00	21.05
2207	N	SER	A	162	75.554	66.431	21.027	1.00	21.51
2209	CA	SER	A	162	76.138	67.660	20.486	1.00	22.08
2211	CB	SER	A	162	77.614	67.492	20.063	1.00	22.37
2214	OG	SER	A	162	77.809	66.365	19.248	1.00	24.18
2216	C	SER	A	162	75.286	68.207	19.336	1.00	21.42
2217	O	SER	A	162	75.142	69.415	19.197	1.00	21.65
2218	N	ALA	A	163	74.700	67.316	18.539	1.00	20.43
2220	CA	ALA	A	163	73.906	67.716	17.379	1.00	20.07
2222	CB	ALA	A	163	73.732	66.523	16.438	1.00	20.07
2226	C	ALA	A	163	72.537	68.265	17.768	1.00	19.77
2227	O	ALA	A	163	71.937	69.041	17.026	1.00	18.96
2228	N	SER	A	164	72.026	67.836	18.922	1.00	19.92
2230	CA	SER	A	164	70.677	68.207	19.366	1.00	19.71
2232	CB	SER	A	164	70.061	67.027	20.112	1.00	20.08
2235	OG	SER	A	164	70.098	65.862	19.285	1.00	21.77
2237	C	SER	A	164	70.655	69.452	20.246	1.00	20.10
2238	O	SER	A	164	69.661	70.210	20.271	1.00	18.98
2239	N	GLY	A	165	71.757	69.676	20.958	1.00	19.76
2241	CA	GLY	A	165	71.846	70.733	21.939	1.00	20.35
2244	C	GLY	A	165	72.244	72.081	21.365	1.00	20.96
2245	O	GLY	A	165	71.982	72.393	20.203	1.00	20.86
2246	N	ILE	A	166	72.900	72.879	22.200	1.00	21.84
2248	CA	ILE	A	166	73.170	74.280	21.914	1.00	22.71
2250	CB	ILE	A	166	73.611	74.975	23.242	1.00	23.10

FIGURE 3 (Cont.)AW

A	B	C	D	E	F	G	H	I	J
2252	CG1	ILE	A	166	73.194	76.437	23.239	1.00	23.87
2255	CD1	ILE	A	166	71.710	76.610	23.444	1.00	23.14
2259	CG2	ILE	A	166	75.109	74.770	23.489	1.00	25.44
2263	C	ILE	A	166	74.197	74.443	20.769	1.00	22.75
2264	O	ILE	A	166	74.206	75.456	20.057	1.00	23.12
2265	N	ALA	A	167	75.027	73.422	20.572	1.00	22.36
2267	CA	ALA	A	167	75.954	73.367	19.451	1.00	22.62
2269	CB	ALA	A	167	77.109	72.455	19.770	1.00	22.85
2273	C	ALA	A	167	75.285	72.916	18.152	1.00	22.34
2274	O	ALA	A	167	75.905	72.963	17.111	1.00	22.65
2275	N	GLY	A	168	74.028	72.488	18.212	1.00	21.57
2277	CA	GLY	A	168	73.304	72.064	17.022	1.00	21.12
2280	C	GLY	A	168	71.883	72.588	16.982	1.00	20.68
2281	O	GLY	A	168	71.665	73.785	16.956	1.00	19.79
2282	N	MET	A	169	70.914	71.682	17.005	1.00	20.95
2284	CA	MET	A	169	69.501	72.019	16.812	1.00	20.87
2286	CB	MET	A	169	68.655	70.757	16.927	1.00	21.21
2289	CG	MET	A	169	67.183	70.922	16.531	1.00	22.91
2292	SD	MET	A	169	66.208	71.479	17.897	1.00	28.34
2293	CE	MET	A	169	66.254	69.967	19.003	1.00	25.97
2297	C	MET	A	169	68.952	73.140	17.721	1.00	20.52
2298	O	MET	A	169	68.310	74.072	17.224	1.00	19.77
2299	N	CYS	A	170	69.200	73.059	19.028	1.00	20.60
2301	CA	CYS	A	170	68.689	74.061	19.977	1.00	20.42
2303	CB	BCYS	A	170	68.958	73.590	21.405	0.35	20.62
2304	CB	ACYS	A	170	68.958	73.668	21.427	0.65	20.89
2309	SG	BCYS	A	170	67.803	74.234	22.609	0.35	20.91
2310	SG	ACYS	A	170	67.804	72.489	22.098	0.65	22.71
2311	C	CYS	A	170	69.332	75.426	19.744	1.00	20.33
2312	O	CYS	A	170	68.665	76.459	19.811	1.00	18.74
2313	N	GLY	A	171	70.650	75.414	19.539	1.00	20.11
2315	CA	GLY	A	171	71.384	76.605	19.172	1.00	20.26
2318	C	GLY	A	171	70.807	77.252	17.932	1.00	20.35
2319	O	GLY	A	171	70.645	78.473	17.877	1.00	19.82
2320	N	GLY	A	172	70.470	76.425	16.948	1.00	20.20
2322	CA	GLY	A	172	69.875	76.891	15.715	1.00	20.43
2325	C	GLY	A	172	68.484	77.441	15.920	1.00	20.51
2326	O	GLY	A	172	68.117	78.435	15.303	1.00	20.93
2327	N	GLN	A	173	67.716	76.816	16.800	1.00	20.70
2329	CA	GLN	A	173	66.397	77.327	17.168	1.00	21.15
2331	CB	GLN	A	173	65.684	76.383	18.149	1.00	21.47
2334	CG	GLN	A	173	65.165	75.072	17.546	1.00	21.62
2337	CD	GLN	A	173	64.102	75.279	16.494	1.00	22.97
2338	OE1	GLN	A	173	64.417	75.656	15.362	1.00	27.11
2339	NE2	GLN	A	173	62.845	75.031	16.850	1.00	22.24
2342	C	GLN	A	173	66.514	78.725	17.794	1.00	21.59
2343	O	GLN	A	173	65.695	79.609	17.513	1.00	22.14
2344	N	ALA	A	174	67.532	78.931	18.622	1.00	21.59
2346	CA	ALA	A	174	67.766	80.245	19.230	1.00	21.99
2348	CB	ALA	A	174	68.847	80.166	20.296	1.00	22.20
2352	C	ALA	A	174	68.152	81.269	18.164	1.00	22.07
2353	O	ALA	A	174	67.683	82.380	18.206	1.00	21.87

FIGURE 3 ~~(Cont.)~~AX

A	B	C	D	E	F	G	H	I	J
2354	N	LEU	A	175	69.001	80.885	17.212	1.00	22.13
2356	CA	LEU	A	175	69.369	81.776	16.106	1.00	23.00
2358	CB	LEU	A	175	70.449	81.144	15.233	1.00	23.09
2361	CG	LEU	A	175	71.824	80.871	15.840	1.00	22.66
2363	CD1	LEU	A	175	72.668	80.085	14.817	1.00	24.29
2367	CD2	LEU	A	175	72.522	82.155	16.235	1.00	22.45
2371	C	LEU	A	175	68.163	82.119	15.240	1.00	23.28
2372	O	LEU	A	175	68.003	83.265	14.805	1.00	23.62
2373	N	ASP	A	176	67.314	81.123	15.002	1.00	23.53
2375	CA	ASP	A	176	66.112	81.280	14.197	1.00	24.49
2377	CB	ASP	A	176	65.382	79.934	14.080	1.00	24.90
2380	CG	ASP	A	176	64.004	80.064	13.491	1.00	25.57
2381	OD1	ASP	A	176	63.830	79.750	12.287	1.00	28.64
2382	OD2	ASP	A	176	63.023	80.441	14.162	1.00	28.54
2383	C	ASP	A	176	65.187	82.320	14.841	1.00	24.97
2384	O	ASP	A	176	64.683	83.222	14.178	1.00	24.47
2385	N	LEU	A	177	64.974	82.168	16.138	1.00	25.23
2387	CA	LEU	A	177	64.127	83.083	16.905	1.00	26.68
2389	CB	LEU	A	177	63.977	82.575	18.343	1.00	26.78
2392	CG	LEU	A	177	62.658	81.902	18.734	1.00	28.22
2394	CD1	LEU	A	177	62.016	81.077	17.633	1.00	29.14
2398	CD2	LEU	A	177	62.892	81.055	19.970	1.00	29.13
2402	C	LEU	A	177	64.686	84.512	16.914	1.00	26.76
2403	O	LEU	A	177	63.936	85.474	16.784	1.00	26.89
2404	N	ASP	A	178	66.002	84.640	17.050	1.00	27.40
2406	CA	ASP	A	178	66.636	85.952	17.078	1.00	28.30
2408	CB	ASP	A	178	68.107	85.827	17.459	1.00	28.53
2411	CG	ASP	A	178	68.753	87.176	17.720	1.00	31.35
2412	OD1	ASP	A	178	69.682	87.571	16.965	1.00	33.39
2413	OD2	ASP	A	178	68.389	87.907	18.667	1.00	33.95
2414	C	ASP	A	178	66.513	86.681	15.734	1.00	28.03
2415	O	ASP	A	178	66.398	87.907	15.689	1.00	27.69
2416	N	ALA	A	179	66.525	85.915	14.648	1.00	27.46
2418	CA	ALA	A	179	66.499	86.467	13.300	1.00	27.69
2420	CB	ALA	A	179	67.174	85.479	12.330	1.00	27.70
2424	C	ALA	A	179	65.089	86.843	12.796	1.00	27.58
2425	O	ALA	A	179	64.946	87.351	11.683	1.00	27.80
2426	N	GLU	A	180	64.057	86.590	13.596	1.00	27.88
2428	CA	GLU	A	180	62.702	87.040	13.277	1.00	28.36
2430	CB	GLU	A	180	61.710	86.633	14.367	1.00	28.57
2433	CG	GLU	A	180	61.415	85.151	14.422	1.00	29.97
2436	CD	GLU	A	180	60.434	84.780	15.517	1.00	32.47
2437	OE1	GLU	A	180	60.070	85.661	16.338	1.00	34.93
2438	OE2	GLU	A	180	60.026	83.598	15.558	1.00	32.41
2439	C	GLU	A	180	62.695	88.560	13.162	1.00	28.40
2440	O	GLU	A	180	63.140	89.252	14.075	1.00	27.70
2441	N	GLY	A	181	62.227	89.057	12.020	1.00	28.55
2443	CA	GLY	A	181	62.105	90.477	11.766	1.00	29.05
2446	C	GLY	A	181	63.391	91.173	11.391	1.00	29.41
2447	O	GLY	A	181	63.379	92.382	11.129	1.00	30.34
2448	N	LYS	A	182	64.501	90.437	11.353	1.00	29.52
2450	CA	LYS	A	182	65.818	91.032	11.137	1.00	29.58

FIGURE 3 (Cont.)AY

A	B	C	D	E	F	G	H	I	J
2452	CB	LYS	A	182	66.807	90.510	12.175	1.00	30.25
2455	CG	LYS	A	182	66.415	90.819	13.604	1.00	31.19
2458	CD	LYS	A	182	67.528	90.474	14.569	1.00	33.42
2461	CE	LYS	A	182	67.168	90.894	16.009	1.00	34.43
2464	NZ	LYS	A	182	65.969	90.178	16.544	1.00	36.01
2468	C	LYS	A	182	66.375	90.797	9.730	1.00	29.61
2469	O	LYS	A	182	67.389	91.383	9.367	1.00	29.31
2470	N	HIS	A	183	65.725	89.944	8.947	1.00	29.18
2472	CA	HIS	A	183	66.098	89.736	7.546	1.00	29.54
2474	CB	HIS	A	183	65.574	90.895	6.688	1.00	29.50
2477	CG	HIS	A	183	64.099	91.086	6.806	1.00	29.04
2478	ND1	HIS	A	183	63.217	90.679	5.835	1.00	29.33
2480	CE1	HIS	A	183	61.982	90.944	6.226	1.00	30.87
2482	NE2	HIS	A	183	62.033	91.486	7.429	1.00	30.77
2484	CD2	HIS	A	183	63.346	91.580	7.816	1.00	30.69
2486	C	HIS	A	183	67.598	89.588	7.410	1.00	29.56
2487	O	HIS	A	183	68.261	90.375	6.732	1.00	29.82
2488	N	VAL	A	184	68.136	88.569	8.067	1.00	29.52
2490	CA	VAL	A	184	69.580	88.461	8.215	1.00	29.40
2492	CB	VAL	A	184	69.976	87.488	9.352	1.00	29.29
2494	CG1	VAL	A	184	69.310	87.904	10.659	1.00	29.32
2498	CG2	VAL	A	184	69.645	86.033	8.998	1.00	28.66
2502	C	VAL	A	184	70.233	88.072	6.886	1.00	29.41
2503	O	VAL	A	184	69.586	87.448	6.037	1.00	29.64
2504	N	PRO	A	185	71.501	88.441	6.701	1.00	29.70
2505	CA	PRO	A	185	72.217	88.146	5.458	1.00	29.74
2507	CB	PRO	A	185	73.565	88.851	5.643	1.00	29.72
2510	CG	PRO	A	185	73.389	89.766	6.777	1.00	30.18
2513	CD	PRO	A	185	72.357	89.168	7.653	1.00	30.09
2516	C	PRO	A	185	72.448	86.659	5.266	1.00	29.95
2517	O	PRO	A	185	72.317	85.896	6.224	1.00	29.23
2518	N	LEU	A	186	72.843	86.279	4.059	1.00	30.11
2520	CA	LEU	A	186	73.010	84.873	3.690	1.00	30.66
2522	CB	LEU	A	186	73.595	84.765	2.281	1.00	30.90
2525	CG	LEU	A	186	73.604	83.417	1.548	1.00	32.07
2527	CD1	LEU	A	186	74.931	82.695	1.750	1.00	34.56
2531	CD2	LEU	A	186	72.438	82.535	1.942	1.00	31.83
2535	C	LEU	A	186	73.875	84.071	4.670	1.00	30.74
2536	O	LEU	A	186	73.472	82.997	5.093	1.00	30.04
2537	N	ASP	A	187	75.058	84.584	5.009	1.00	30.98
2539	CA	ASP	A	187	75.951	83.903	5.945	1.00	31.77
2541	CB	ASP	A	187	77.278	84.667	6.143	1.00	32.58
2544	CG	ASP	A	187	77.097	86.128	6.641	1.00	34.74
2545	OD1	ASP	A	187	75.963	86.630	6.812	1.00	37.70
2546	OD2	ASP	A	187	78.079	86.866	6.881	1.00	39.45
2547	C	ASP	A	187	75.295	83.578	7.301	1.00	31.43
2548	O	ASP	A	187	75.516	82.494	7.847	1.00	31.36
2549	N	ALA	A	188	74.493	84.505	7.823	1.00	30.71
2551	CA	ALA	A	188	73.781	84.297	9.082	1.00	30.32
2553	CB	ALA	A	188	73.271	85.624	9.641	1.00	30.46
2557	C	ALA	A	188	72.627	83.331	8.870	1.00	29.80
2558	O	ALA	A	188	72.328	82.505	9.731	1.00	28.47

FIGURE 3 (Cont.)AZ

A	B	C	D	E	F	G	H	I	J
2559	N	LEU	A	189	71.990	83.427	7.708	1.00	29.23
2561	CA	LEU	A	189	70.902	82.529	7.358	1.00	29.70
2563	CB	LEU	A	189	70.360	82.867	5.971	1.00	30.15
2566	CG	LEU	A	189	68.870	83.128	5.772	1.00	31.79
2568	CD1	LEU	A	189	68.545	82.912	4.280	1.00	32.57
2572	CD2	LEU	A	189	67.958	82.296	6.672	1.00	32.39
2576	C	LEU	A	189	71.397	81.077	7.356	1.00	29.25
2577	O	LEU	A	189	70.766	80.182	7.923	1.00	27.68
2578	N	GLU	A	190	72.539	80.867	6.712	1.00	28.91
2580	CA	GLU	A	190	73.138	79.547	6.604	1.00	28.82
2582	CB	GLU	A	190	74.362	79.609	5.697	1.00	29.44
2585	CG	GLU	A	190	74.926	78.249	5.322	1.00	31.65
2588	CD	GLU	A	190	76.119	78.345	4.382	1.00	35.05
2589	OE1	GLU	A	190	76.048	79.127	3.405	1.00	36.65
2590	OE2	GLU	A	190	77.126	77.631	4.625	1.00	37.41
2591	C	GLU	A	190	73.524	78.996	7.972	1.00	28.22
2592	O	GLU	A	190	73.406	77.807	8.220	1.00	27.03
2593	N	ARG	A	191	74.001	79.866	8.856	1.00	27.79
2595	CA	ARG	A	191	74.342	79.454	10.210	1.00	27.69
2597	CB	ARG	A	191	75.021	80.585	10.988	1.00	28.29
2600	CG	ARG	A	191	76.429	80.908	10.483	1.00	32.30
2603	CD	ARG	A	191	77.323	81.682	11.474	1.00	35.96
2606	NE	ARG	A	191	78.509	80.902	11.831	1.00	39.49
2608	CZ	ARG	A	191	79.520	80.619	11.005	1.00	42.00
2609	NH1	ARG	A	191	79.524	81.054	9.748	1.00	43.12
2612	NH2	ARG	A	191	80.539	79.889	11.440	1.00	42.49
2615	C	ARG	A	191	73.100	78.970	10.948	1.00	26.20
2616	O	ARG	A	191	73.153	77.952	11.634	1.00	25.47
2617	N	ILE	A	192	71.985	79.681	10.787	1.00	25.12
2619	CA	ILE	A	192	70.719	79.254	11.387	1.00	24.45
2621	CB	ILE	A	192	69.546	80.183	11.009	1.00	24.28
2623	CG1	ILE	A	192	69.717	81.579	11.619	1.00	25.03
2626	CD1	ILE	A	192	68.851	82.624	10.981	1.00	25.02
2630	CG2	ILE	A	192	68.222	79.577	11.474	1.00	24.54
2634	C	ILE	A	192	70.385	77.842	10.906	1.00	24.27
2635	O	ILE	A	192	70.205	76.928	11.699	1.00	23.05
2636	N	HIS	A	193	70.289	77.701	9.590	1.00	23.44
2638	CA	HIS	A	193	69.789	76.477	8.976	1.00	23.31
2640	CB	HIS	A	193	69.573	76.731	7.485	1.00	23.43
2643	CG	HIS	A	193	68.349	77.547	7.209	1.00	24.48
2644	ND1	HIS	A	193	67.494	77.964	8.208	1.00	25.73
2646	CE1	HIS	A	193	66.480	78.623	7.675	1.00	26.42
2648	NE2	HIS	A	193	66.659	78.669	6.367	1.00	25.37
2650	CD2	HIS	A	193	67.817	77.999	6.052	1.00	25.77
2652	C	HIS	A	193	70.678	75.264	9.230	1.00	22.37
2653	O	HIS	A	193	70.179	74.181	9.534	1.00	22.47
2654	N	ARG	A	194	71.986	75.445	9.128	1.00	21.53
2656	CA	ARG	A	194	72.919	74.362	9.391	1.00	21.47
2658	CB	ARG	A	194	74.358	74.778	9.120	1.00	20.83
2661	CG	ARG	A	194	74.700	74.835	7.656	1.00	21.22
2664	CD	ARG	A	194	76.180	74.847	7.423	1.00	22.88
2667	NE	ARG	A	194	76.501	75.077	6.022	1.00	24.27

FIGURE 3 ~~(Cont.)~~BA

A	B	C	D	E	F	G	H	I	J
2669	CZ	ARG	A	194	76.459	74.147	5.092	1.00	25.12
2670	NH1	ARG	A	194	76.120	72.904	5.398	1.00	25.42
2673	NH2	ARG	A	194	76.784	74.455	3.840	1.00	28.83
2676	C	ARG	A	194	72.780	73.872	10.829	1.00	21.18
2677	O	ARG	A	194	72.861	72.681	11.071	1.00	20.79
2678	N	HIS	A	195	72.583	74.777	11.784	1.00	21.00
2680	CA	HIS	A	195	72.436	74.337	13.171	1.00	21.63
2682	CB	HIS	A	195	72.773	75.458	14.158	1.00	21.62
2685	CG	HIS	A	195	74.232	75.787	14.215	1.00	24.46
2686	ND1	HIS	A	195	74.944	75.833	15.394	1.00	28.06
2688	CE1	HIS	A	195	76.201	76.148	15.134	1.00	28.87
2690	NE2	HIS	A	195	76.330	76.304	13.831	1.00	29.50
2692	CD2	HIS	A	195	75.113	76.086	13.233	1.00	27.40
2694	C	HIS	A	195	71.050	73.751	13.451	1.00	21.00
2695	O	HIS	A	195	70.948	72.646	13.985	1.00	20.86
2696	N	LYS	A	196	69.985	74.462	13.087	1.00	20.63
2698	CA	LYS	A	196	68.642	74.022	13.489	1.00	20.10
2700	CB	LYS	A	196	67.590	75.123	13.367	1.00	19.88
2703	CG	LYS	A	196	66.987	75.363	11.997	1.00	19.59
2706	CD	LYS	A	196	65.944	76.473	12.065	1.00	19.02
2709	CE	LYS	A	196	65.416	76.847	10.672	1.00	18.63
2712	NZ	LYS	A	196	64.064	77.494	10.673	1.00	19.09
2716	C	LYS	A	196	68.215	72.756	12.758	1.00	20.00
2717	O	LYS	A	196	67.491	71.960	13.307	1.00	20.23
2718	N	THR	A	197	68.705	72.557	11.539	1.00	19.63
2720	CA	THR	A	197	68.278	71.433	10.726	1.00	19.13
2722	CB	THR	A	197	67.408	71.938	9.580	1.00	19.35
2724	OG1	THR	A	197	66.166	72.400	10.127	1.00	18.33
2726	CG2	THR	A	197	67.021	70.812	8.618	1.00	18.67
2730	C	THR	A	197	69.413	70.554	10.226	1.00	19.03
2731	O	THR	A	197	69.275	69.332	10.223	1.00	18.17
2732	N	GLY	A	198	70.522	71.167	9.812	1.00	19.30
2734	CA	GLY	A	198	71.667	70.421	9.316	1.00	19.16
2737	C	GLY	A	198	72.260	69.466	10.329	1.00	19.28
2738	O	GLY	A	198	72.580	68.330	9.987	1.00	19.12
2739	N	ALA	A	199	72.371	69.910	11.576	1.00	19.18
2741	CA	ALA	A	199	73.129	69.182	12.585	1.00	19.36
2743	CB	ALA	A	199	73.245	70.005	13.861	1.00	19.70
2747	C	ALA	A	199	72.505	67.816	12.897	1.00	19.34
2748	O	ALA	A	199	73.224	66.830	13.057	1.00	19.28
2749	N	LEU	A	200	71.177	67.768	12.994	1.00	19.51
2751	CA	LEU	A	200	70.476	66.522	13.302	1.00	19.63
2753	CB	LEU	A	200	69.016	66.775	13.700	1.00	19.77
2756	CG	LEU	A	200	68.261	65.516	14.183	1.00	20.34
2758	CD1	LEU	A	200	68.918	64.931	15.431	1.00	20.63
2762	CD2	LEU	A	200	66.799	65.855	14.449	1.00	20.55
2766	C	LEU	A	200	70.514	65.563	12.125	1.00	19.55
2767	O	LEU	A	200	70.590	64.336	12.312	1.00	19.72
2768	N	ILE	A	201	70.462	66.114	10.919	1.00	19.19
2770	CA	ILE	A	201	70.556	65.299	9.706	1.00	19.51
2772	CB	ILE	A	201	70.178	66.143	8.471	1.00	19.64
2774	CG1	ILE	A	201	68.659	66.197	8.372	1.00	20.21

FIGURE 3 (Cont.)BB

A	B	C	D	E	F	G	H	I	J
2777	CD1	ILE	A	201	68.149	67.249	7.449	1.00	21.65
2781	CG2	ILE	A	201	70.782	65.578	7.169	1.00	20.92
2785	C	ILE	A	201	71.941	64.661	9.604	1.00	19.17
2786	O	ILE	A	201	72.066	63.504	9.227	1.00	18.77
2787	N	ARG	A	202	72.970	65.420	9.963	1.00	19.39
2789	CA	ARG	A	202	74.323	64.891	10.001	1.00	19.72
2791	CB	ARG	A	202	75.343	66.008	10.148	1.00	20.03
2794	CG	ARG	A	202	76.774	65.526	10.119	1.00	21.06
2797	CD	ARG	A	202	77.777	66.638	10.165	1.00	20.98
2800	NE	ARG	A	202	77.824	67.265	11.473	1.00	23.53
2802	CZ	ARG	A	202	78.617	68.294	11.789	1.00	25.30
2803	NH1	ARG	A	202	78.580	68.800	13.012	1.00	23.66
2806	NH2	ARG	A	202	79.445	68.815	10.891	1.00	26.69
2809	C	ARG	A	202	74.453	63.843	11.113	1.00	19.73
2810	O	ARG	A	202	75.153	62.859	10.935	1.00	19.84
2811	N	ALA	A	203	73.741	64.027	12.226	1.00	19.24
2813	CA	ALA	A	203	73.713	63.009	13.276	1.00	18.65
2815	CB	ALA	A	203	73.001	63.513	14.517	1.00	19.04
2819	C	ALA	A	203	73.097	61.696	12.824	1.00	18.20
2820	O	ALA	A	203	73.582	60.644	13.210	1.00	18.83
2821	N	ALA	A	204	72.025	61.740	12.043	1.00	18.01
2823	CA	ALA	A	204	71.441	60.524	11.485	1.00	18.08
2825	CB	ALA	A	204	70.268	60.868	10.588	1.00	18.17
2829	C	ALA	A	204	72.481	59.738	10.700	1.00	18.04
2830	O	ALA	A	204	72.645	58.522	10.879	1.00	17.73
2831	N	VAL	A	205	73.170	60.430	9.809	1.00	17.87
2833	CA	VAL	A	205	74.174	59.786	8.990	1.00	18.48
2835	CB	VAL	A	205	74.659	60.714	7.874	1.00	18.22
2837	CG1	VAL	A	205	75.791	60.079	7.109	1.00	18.92
2841	CG2	VAL	A	205	73.476	61.057	6.930	1.00	17.58
2845	C	VAL	A	205	75.314	59.238	9.852	1.00	18.69
2846	O	VAL	A	205	75.716	58.086	9.677	1.00	20.23
2847	N	ARG	A	206	75.783	60.032	10.808	1.00	18.74
2849	CA	ARG	A	206	76.862	59.629	11.702	1.00	18.96
2851	CB	ARG	A	206	77.274	60.778	12.615	1.00	18.76
2854	CG	ARG	A	206	78.157	61.792	11.948	1.00	19.71
2857	CD	ARG	A	206	78.477	63.008	12.803	1.00	19.66
2860	NE	ARG	A	206	79.481	63.857	12.167	1.00	21.03
2862	CZ	ARG	A	206	80.008	64.936	12.737	1.00	22.60
2863	NH1	ARG	A	206	79.659	65.289	13.965	1.00	22.08
2866	NH2	ARG	A	206	80.903	65.660	12.079	1.00	21.63
2869	C	ARG	A	206	76.481	58.427	12.549	1.00	19.18
2870	O	ARG	A	206	77.283	57.530	12.757	1.00	18.61
2871	N	LEU	A	207	75.244	58.394	13.014	1.00	19.73
2873	CA	LEU	A	207	74.790	57.288	13.850	1.00	20.29
2875	CB	LEU	A	207	73.426	57.600	14.481	1.00	20.21
2878	CG	LEU	A	207	73.432	58.067	15.944	1.00	21.69
2880	CD1	LEU	A	207	74.453	59.147	16.210	1.00	22.70
2884	CD2	LEU	A	207	72.044	58.554	16.298	1.00	23.52
2888	C	LEU	A	207	74.715	56.013	13.013	1.00	20.31
2889	O	LEU	A	207	75.049	54.941	13.486	1.00	19.90
2890	N	GLY	A	208	74.273	56.131	11.772	1.00	20.46

FIGURE 3 ~~(Cont.)~~BC

A	B	C	D	E	F	G	H	I	J
2892	CA	GLY	A	208	74.297	55.000	10.861	1.00	21.15
2895	C	GLY	A	208	75.703	54.457	10.656	1.00	21.20
2896	O	GLY	A	208	75.933	53.240	10.737	1.00	22.15
2897	N	ALA	A	209	76.643	55.362	10.419	1.00	21.27
2899	CA	ALA	A	209	78.046	55.006	10.215	1.00	22.05
2901	CB	ALA	A	209	78.813	56.193	9.733	1.00	21.96
2905	C	ALA	A	209	78.700	54.419	11.480	1.00	22.41
2906	O	ALA	A	209	79.383	53.398	11.411	1.00	22.53
2907	N	LEU	A	210	78.471	55.041	12.635	1.00	22.29
2909	CA	LEU	A	210	79.090	54.580	13.877	1.00	22.51
2911	CB	LEU	A	210	78.775	55.522	15.039	1.00	22.37
2914	CG	LEU	A	210	79.513	56.853	14.977	1.00	22.40
2916	CD1	LEU	A	210	78.845	57.900	15.863	1.00	22.42
2920	CD2	LEU	A	210	81.004	56.689	15.372	1.00	22.32
2924	C	LEU	A	210	78.642	53.168	14.213	1.00	23.22
2925	O	LEU	A	210	79.383	52.408	14.830	1.00	23.30
2926	N	SER	A	211	77.430	52.809	13.786	1.00	24.01
2928	CA	SER	A	211	76.914	51.469	13.999	1.00	24.10
2930	CB	SER	A	211	75.478	51.347	13.496	1.00	24.10
2933	OG	SER	A	211	75.459	51.162	12.104	1.00	25.59
2935	C	SER	A	211	77.764	50.397	13.335	1.00	24.24
2936	O	SER	A	211	77.746	49.254	13.778	1.00	23.60
2937	N	ALA	A	212	78.464	50.782	12.269	1.00	24.79
2939	CA	ALA	A	212	79.332	49.906	11.496	1.00	25.88
2941	CB	ALA	A	212	79.361	50.376	10.050	1.00	26.06
2945	C	ALA	A	212	80.762	49.837	12.044	1.00	26.25
2946	O	ALA	A	212	81.602	49.130	11.490	1.00	27.04
2947	N	GLY	A	213	81.051	50.586	13.100	1.00	26.38
2949	CA	GLY	A	213	82.373	50.574	13.692	1.00	27.08
2952	C	GLY	A	213	83.427	51.209	12.809	1.00	27.54
2953	O	GLY	A	213	83.193	52.242	12.199	1.00	27.58
2954	N	ASP	A	214	84.584	50.570	12.718	1.00	28.92
2956	CA	ASP	A	214	85.758	51.188	12.105	1.00	29.67
2958	CB	ASP	A	214	86.993	50.294	12.281	1.00	30.31
2961	CG	ASP	A	214	87.596	50.413	13.666	1.00	33.03
2962	OD1	ASP	A	214	88.445	49.568	14.020	1.00	37.45
2963	OD2	ASP	A	214	87.285	51.318	14.478	1.00	35.85
2964	C	ASP	A	214	85.530	51.523	10.650	1.00	29.40
2965	O	ASP	A	214	85.907	52.596	10.203	1.00	29.23
2966	N	LYS	A	215	84.879	50.625	9.921	1.00	29.50
2968	CA	LYS	A	215	84.593	50.862	8.505	1.00	29.92
2970	CB	LYS	A	215	84.019	49.610	7.839	1.00	30.45
2973	CG	LYS	A	215	85.103	48.766	7.182	1.00	33.43
2976	CD	LYS	A	215	84.685	47.310	6.964	1.00	36.17
2979	CE	LYS	A	215	85.888	46.439	6.568	1.00	37.55
2982	NZ	LYS	A	215	85.967	45.213	7.416	1.00	39.13
2986	C	LYS	A	215	83.672	52.076	8.312	1.00	29.02
2987	O	LYS	A	215	83.851	52.860	7.384	1.00	27.84
2988	N	GLY	A	216	82.696	52.241	9.198	1.00	28.66
2990	CA	GLY	A	216	81.855	53.429	9.162	1.00	28.17
2993	C	GLY	A	216	82.647	54.692	9.471	1.00	27.77
2994	O	GLY	A	216	82.503	55.719	8.812	1.00	27.08

FIGURE 3 (Cont.)BD

A	B	C	D	E	F	G	H	I	J
2995	N	ARG	A	217	83.498	54.609	10.482	1.00	27.98
2997	CA	ARG	A	217	84.306	55.751	10.900	1.00	28.29
2999	CB	ARG	A	217	85.165	55.391	12.106	1.00	28.55
3002	CG	ARG	A	217	84.449	55.520	13.428	1.00	28.34
3005	CD	ARG	A	217	85.328	55.173	14.580	1.00	29.33
3008	NE	ARG	A	217	84.577	55.110	15.826	1.00	29.90
3010	CZ	ARG	A	217	84.375	56.148	16.637	1.00	29.01
3011	NH1	ARG	A	217	84.836	57.359	16.334	1.00	29.10
3014	NH2	ARG	A	217	83.671	55.980	17.743	1.00	28.00
3017	C	ARG	A	217	85.201	56.266	9.783	1.00	28.80
3018	O	ARG	A	217	85.367	57.476	9.645	1.00	28.97
3019	N	ARG	A	218	85.752	55.354	8.978	1.00	29.00
3021	CA	ARG	A	218	86.622	55.726	7.853	1.00	29.76
3023	CB	ARG	A	218	87.268	54.483	7.223	1.00	30.54
3026	CG	ARG	A	218	88.351	53.812	8.069	1.00	33.89
3029	CD	ARG	A	218	88.273	52.280	8.115	1.00	38.26
3032	NE	ARG	A	218	88.914	51.617	6.975	1.00	41.13
3034	CZ	ARG	A	218	88.318	51.290	5.817	1.00	44.61
3035	NH1	ARG	A	218	89.023	50.681	4.862	1.00	46.06
3038	NH2	ARG	A	218	87.037	51.564	5.587	1.00	45.97
3041	C	ARG	A	218	85.866	56.481	6.765	1.00	29.10
3042	O	ARG	A	218	86.460	57.283	6.034	1.00	29.09
3043	N	ALA	A	219	84.565	56.209	6.646	1.00	27.99
3045	CA	ALA	A	219	83.720	56.894	5.669	1.00	27.60
3047	CB	ALA	A	219	82.532	56.030	5.313	1.00	27.48
3051	C	ALA	A	219	83.234	58.253	6.142	1.00	27.24
3052	O	ALA	A	219	82.710	59.018	5.344	1.00	26.75
3053	N	LEU	A	220	83.394	58.543	7.433	1.00	27.30
3055	CA	LEU	A	220	82.807	59.736	8.036	1.00	27.51
3057	CB	LEU	A	220	83.061	59.804	9.546	1.00	27.81
3060	CG	LEU	A	220	82.127	58.960	10.416	1.00	29.69
3062	CD1	LEU	A	220	82.573	59.004	11.889	1.00	30.50
3066	CD2	LEU	A	220	80.677	59.411	10.271	1.00	30.60
3070	C	LEU	A	220	83.226	61.045	7.400	1.00	26.87
3071	O	LEU	A	220	82.380	61.901	7.232	1.00	27.16
3072	N	PRO	A	221	84.502	61.248	7.067	1.00	26.59
3073	CA	PRO	A	221	84.879	62.502	6.399	1.00	26.30
3075	CB	PRO	A	221	86.349	62.269	6.006	1.00	26.54
3078	CG	PRO	A	221	86.853	61.366	7.081	1.00	27.08
3081	CD	PRO	A	221	85.685	60.415	7.352	1.00	26.58
3084	C	PRO	A	221	83.996	62.758	5.195	1.00	25.66
3085	O	PRO	A	221	83.479	63.859	5.044	1.00	26.22
3086	N	VAL	A	222	83.770	61.735	4.381	1.00	24.71
3088	CA	VAL	A	222	82.965	61.910	3.181	1.00	24.34
3090	CB	VAL	A	222	83.272	60.835	2.139	1.00	24.09
3092	CG1	VAL	A	222	82.302	60.927	0.999	1.00	23.94
3096	CG2	VAL	A	222	84.718	60.988	1.655	1.00	25.44
3100	C	VAL	A	222	81.465	61.955	3.470	1.00	23.78
3101	O	VAL	A	222	80.754	62.771	2.885	1.00	23.40
3102	N	LEU	A	223	80.978	61.096	4.362	1.00	23.25
3104	CA	LEU	A	223	79.552	61.118	4.707	1.00	22.90
3106	CB	LEU	A	223	79.179	59.955	5.627	1.00	23.13

FIGURE 3 ~~(Cont.)~~BE

A	B	C	D	E	F	G	H	I	J
3109	CG	LEU	A	223	79.130	58.583	4.947	1.00	22.78
3111	CD1	LEU	A	223	79.022	57.462	5.987	1.00	23.57
3115	CD2	LEU	A	223	77.991	58.484	3.975	1.00	23.72
3119	C	LEU	A	223	79.159	62.441	5.346	1.00	23.02
3120	O	LEU	A	223	78.023	62.903	5.182	1.00	22.74
3121	N	ASP	A	224	80.081	63.036	6.093	1.00	23.24
3123	CA	ASP	A	224	79.838	64.328	6.722	1.00	23.61
3125	CB	ASP	A	224	81.028	64.753	7.588	1.00	23.94
3128	CG	ASP	A	224	81.009	64.118	8.974	1.00	25.27
3129	OD1	ASP	A	224	79.961	63.561	9.379	1.00	25.31
3130	OD2	ASP	A	224	81.989	64.158	9.749	1.00	27.02
3131	C	ASP	A	224	79.568	65.385	5.654	1.00	23.60
3132	O	ASP	A	224	78.630	66.175	5.772	1.00	22.89
3133	N	LYS	A	225	80.373	65.377	4.599	1.00	23.58
3135	CA	LYS	A	225	80.234	66.391	3.557	1.00	24.32
3137	CB	LYS	A	225	81.439	66.381	2.594	1.00	24.94
3140	CG	LYS	A	225	82.825	66.478	3.298	1.00	27.64
3143	CD	LYS	A	225	83.113	67.828	4.009	1.00	31.84
3146	CE	LYS	A	225	83.516	67.719	5.546	1.00	32.28
3149	NZ	LYS	A	225	84.063	66.374	6.064	1.00	30.63
3153	C	LYS	A	225	78.901	66.207	2.842	1.00	23.43
3154	O	LYS	A	225	78.205	67.177	2.548	1.00	23.79
3155	N	TYR	A	226	78.521	64.955	2.612	1.00	22.64
3157	CA	TYR	A	226	77.214	64.632	2.063	1.00	21.59
3159	CB	TYR	A	226	77.075	63.114	1.881	1.00	21.93
3162	CG	TYR	A	226	75.645	62.633	1.753	1.00	20.62
3163	CD1	TYR	A	226	75.021	62.606	0.523	1.00	21.37
3165	CE1	TYR	A	226	73.736	62.160	0.386	1.00	20.90
3167	CZ	TYR	A	226	73.030	61.727	1.487	1.00	20.66
3168	OH	TYR	A	226	71.737	61.289	1.311	1.00	21.67
3170	CE2	TYR	A	226	73.617	61.727	2.730	1.00	21.12
3172	CD2	TYR	A	226	74.933	62.174	2.862	1.00	20.69
3174	C	TYR	A	226	76.098	65.121	2.979	1.00	21.19
3175	O	TYR	A	226	75.156	65.754	2.523	1.00	21.30
3176	N	ALA	A	227	76.208	64.804	4.261	1.00	20.68
3178	CA	ALA	A	227	75.173	65.126	5.240	1.00	20.41
3180	CB	ALA	A	227	75.503	64.513	6.581	1.00	20.07
3184	C	ALA	A	227	75.007	66.627	5.390	1.00	20.36
3185	O	ALA	A	227	73.893	67.123	5.485	1.00	19.95
3186	N	GLU	A	228	76.132	67.326	5.407	1.00	20.85
3188	CA	GLU	A	228	76.160	68.786	5.503	1.00	21.65
3190	CB	GLU	A	228	77.601	69.285	5.581	1.00	21.59
3193	CG	GLU	A	228	78.225	69.020	6.940	1.00	23.51
3196	CD	GLU	A	228	79.737	68.868	6.911	1.00	25.72
3197	OE1	GLU	A	228	80.292	68.333	7.899	1.00	25.16
3198	OE2	GLU	A	228	80.367	69.272	5.910	1.00	28.53
3199	C	GLU	A	228	75.411	69.428	4.340	1.00	21.53
3200	O	GLU	A	228	74.644	70.370	4.532	1.00	22.09
3201	N	SER	A	229	75.600	68.899	3.141	1.00	21.49
3203	CA	SER	A	229	74.922	69.459	1.985	1.00	21.57
3205	CB	SER	A	229	75.598	69.036	0.695	1.00	21.17
3208	OG	SER	A	229	76.870	69.647	0.589	1.00	22.38

FIGURE 3 (Cont.)BF

A	B	C	D	E	F	G	H	I	J
3210	C	SER	A	229	73.432	69.119	1.967	1.00	21.32
3211	O	SER	A	229	72.629	69.993	1.719	1.00	20.51
3212	N	ILE	A	230	73.044	67.871	2.238	1.00	21.52
3214	CA	ILE	A	230	71.610	67.562	2.236	1.00	21.70
3216	CB	ILE	A	230	71.318	66.049	2.154	1.00	21.58
3218	CG1	ILE	A	230	71.881	65.279	3.347	1.00	22.85
3221	CD1	ILE	A	230	71.069	64.038	3.669	1.00	22.81
3225	CG2	ILE	A	230	71.815	65.486	0.849	1.00	21.97
3229	C	ILE	A	230	70.874	68.190	3.421	1.00	21.12
3230	O	ILE	A	230	69.684	68.467	3.337	1.00	21.31
3231	N	GLY	A	231	71.583	68.412	4.520	1.00	21.08
3233	CA	GLY	A	231	70.983	68.977	5.714	1.00	21.32
3236	C	GLY	A	231	70.607	70.441	5.534	1.00	21.14
3237	O	GLY	A	231	69.514	70.877	5.917	1.00	21.86
3238	N	LEU	A	232	71.513	71.205	4.939	1.00	21.35
3240	CA	LEU	A	232	71.214	72.583	4.595	1.00	21.18
3242	CB	LEU	A	232	72.467	73.318	4.127	1.00	21.49
3245	CG	LEU	A	232	72.250	74.769	3.712	1.00	21.63
3247	CD1	LEU	A	232	71.601	75.564	4.829	1.00	22.56
3251	CD2	LEU	A	232	73.571	75.361	3.320	1.00	23.37
3255	C	LEU	A	232	70.134	72.604	3.521	1.00	20.95
3256	O	LEU	A	232	69.171	73.324	3.659	1.00	20.57
3257	N	ALA	A	233	70.270	71.766	2.488	1.00	20.80
3259	CA	ALA	A	233	69.271	71.677	1.424	1.00	20.94
3261	CB	ALA	A	233	69.674	70.639	0.373	1.00	21.23
3265	C	ALA	A	233	67.885	71.350	1.966	1.00	20.81
3266	O	ALA	A	233	66.878	71.812	1.442	1.00	20.67
3267	N	PHE	A	234	67.840	70.554	3.029	1.00	20.67
3269	CA	PHE	A	234	66.568	70.166	3.634	1.00	20.70
3271	CB	PHE	A	234	66.798	69.201	4.785	1.00	20.78
3274	CG	PHE	A	234	65.600	68.375	5.131	1.00	22.14
3275	CD1	PHE	A	234	65.546	67.041	4.768	1.00	23.74
3277	CE1	PHE	A	234	64.455	66.267	5.103	1.00	25.17
3279	CZ	PHE	A	234	63.407	66.817	5.797	1.00	23.85
3281	CE2	PHE	A	234	63.462	68.143	6.173	1.00	23.26
3283	CD2	PHE	A	234	64.551	68.907	5.851	1.00	21.11
3285	C	PHE	A	234	65.812	71.378	4.147	1.00	20.30
3286	O	PHE	A	234	64.590	71.496	3.939	1.00	19.63
3287	N	GLN	A	235	66.523	72.269	4.835	1.00	20.63
3289	CA	GLN	A	235	65.874	73.456	5.381	1.00	21.12
3291	CB	GLN	A	235	66.699	74.091	6.503	1.00	21.39
3294	CG	GLN	A	235	65.944	75.205	7.276	1.00	21.45
3297	CD	GLN	A	235	64.668	74.715	7.926	1.00	23.00
3298	OE1	GLN	A	235	64.650	73.654	8.548	1.00	23.23
3299	NE2	GLN	A	235	63.595	75.490	7.795	1.00	20.99
3302	C	GLN	A	235	65.546	74.494	4.300	1.00	21.77
3303	O	GLN	A	235	64.511	75.148	4.375	1.00	22.39
3304	N	VAL	A	236	66.402	74.641	3.299	1.00	22.51
3306	CA	VAL	A	236	66.066	75.543	2.184	1.00	22.92
3308	CB	VAL	A	236	67.260	75.840	1.212	1.00	23.27
3310	CG1	VAL	A	236	68.054	74.664	0.922	1.00	26.25
3314	CG2	VAL	A	236	66.794	76.486	-0.102	1.00	23.71

FIGURE 3 ~~(Cont.)~~BG

A	B	C	D	E	F	G	H	I	J
3318	C	VAL	A	236	64.794	75.075	1.478	1.00	22.84
3319	O	VAL	A	236	63.936	75.893	1.150	1.00	22.34
3320	N	GLN	A	237	64.635	73.761	1.307	1.00	23.02
3322	CA	GLN	A	237	63.413	73.222	0.738	1.00	23.04
3324	CB	GLN	A	237	63.538	71.727	0.418	1.00	23.87
3327	CG	GLN	A	237	62.276	71.128	-0.198	1.00	25.59
3330	CD	GLN	A	237	62.058	71.593	-1.623	1.00	29.42
3331	OE1	GLN	A	237	62.818	72.426	-2.133	1.00	30.57
3332	NE2	GLN	A	237	61.025	71.053	-2.275	1.00	28.29
3335	C	GLN	A	237	62.241	73.441	1.671	1.00	22.23
3336	O	GLN	A	237	61.140	73.709	1.213	1.00	22.37
3337	N	ASP	A	238	62.467	73.315	2.977	1.00	21.60
3339	CA	ASP	A	238	61.409	73.564	3.954	1.00	21.14
3341	CB	ASP	A	238	61.898	73.263	5.372	1.00	20.81
3344	CG	ASP	A	238	60.808	73.400	6.393	1.00	20.15
3345	OD1	ASP	A	238	59.877	72.588	6.376	1.00	22.40
3346	OD2	ASP	A	238	60.774	74.310	7.250	1.00	23.26
3347	C	ASP	A	238	60.904	75.018	3.848	1.00	21.37
3348	O	ASP	A	238	59.701	75.260	3.866	1.00	21.86
3349	N	ASP	A	239	61.820	75.966	3.694	1.00	21.89
3351	CA	ASP	A	239	61.446	77.379	3.534	1.00	22.75
3353	CB	ASP	A	239	62.674	78.275	3.478	1.00	22.66
3356	CG	ASP	A	239	63.436	78.375	4.789	1.00	23.92
3357	OD1	ASP	A	239	62.965	77.899	5.859	1.00	26.27
3358	OD2	ASP	A	239	64.542	78.966	4.821	1.00	23.49
3359	C	ASP	A	239	60.679	77.596	2.219	1.00	23.14
3360	O	ASP	A	239	59.719	78.357	2.158	1.00	23.09
3361	N	ILE	A	240	61.129	76.934	1.162	1.00	24.22
3363	CA	ILE	A	240	60.507	77.067	-0.150	1.00	24.50
3365	CB	ILE	A	240	61.358	76.356	-1.230	1.00	24.79
3367	CG1	ILE	A	240	62.593	77.200	-1.545	1.00	25.00
3370	CD1	ILE	A	240	63.697	76.444	-2.246	1.00	25.62
3374	CG2	ILE	A	240	60.548	76.118	-2.518	1.00	24.83
3378	C	ILE	A	240	59.094	76.529	-0.095	1.00	24.74
3379	O	ILE	A	240	58.168	77.162	-0.598	1.00	24.41
3380	N	LEU	A	241	58.920	75.380	0.561	1.00	24.90
3382	CA	LEU	A	241	57.608	74.763	0.702	1.00	25.47
3384	CB	LEU	A	241	57.721	73.376	1.346	1.00	25.41
3387	CG	LEU	A	241	58.364	72.296	0.469	1.00	26.20
3389	CD1	LEU	A	241	58.592	71.012	1.275	1.00	26.19
3393	CD2	LEU	A	241	57.523	72.032	-0.762	1.00	26.28
3397	C	LEU	A	241	56.677	75.637	1.517	1.00	25.82
3398	O	LEU	A	241	55.463	75.646	1.296	1.00	26.02
3399	N	ASP	A	242	57.238	76.375	2.461	1.00	26.06
3401	CA	ASP	A	242	56.422	77.233	3.298	1.00	27.02
3403	CB	ASP	A	242	57.239	77.832	4.426	1.00	26.69
3406	CG	ASP	A	242	56.390	78.176	5.607	1.00	28.82
3407	OD1	ASP	A	242	55.886	79.319	5.636	1.00	29.75
3408	OD2	ASP	A	242	56.148	77.365	6.534	1.00	31.49
3409	C	ASP	A	242	55.765	78.333	2.458	1.00	27.65
3410	O	ASP	A	242	54.622	78.689	2.698	1.00	28.08
3411	N	VAL	A	243	56.481	78.823	1.454	1.00	28.57

FIGURE 3 (Cont.)BH

A	B	C	D	E	F	G	H	I	J
3413	CA	VAL	A	243	55.949	79.838	0.542	1.00	29.59
3415	CB	VAL	A	243	57.091	80.577	-0.188	1.00	29.49
3417	CG1	VAL	A	243	56.537	81.656	-1.140	1.00	29.98
3421	CG2	VAL	A	243	58.062	81.200	0.825	1.00	29.51
3425	C	VAL	A	243	54.951	79.248	-0.477	1.00	30.63
3426	O	VAL	A	243	53.791	79.669	-0.525	1.00	30.78
3427	N	VAL	A	244	55.388	78.253	-1.250	1.00	31.44
3429	CA	VAL	A	244	54.642	77.785	-2.427	1.00	32.17
3431	CB	VAL	A	244	55.605	77.525	-3.617	1.00	32.40
3433	CG1	VAL	A	244	56.588	78.680	-3.768	1.00	32.66
3437	CG2	VAL	A	244	56.349	76.185	-3.462	1.00	32.82
3441	C	VAL	A	244	53.766	76.543	-2.233	1.00	32.47
3442	O	VAL	A	244	52.963	76.204	-3.110	1.00	32.70
3443	N	GLY	A	245	53.915	75.854	-1.105	1.00	32.77
3445	CA	GLY	A	245	53.200	74.611	-0.879	1.00	33.14
3448	C	GLY	A	245	51.784	74.871	-0.407	1.00	33.82
3449	O	GLY	A	245	51.515	75.920	0.162	1.00	34.10
3450	N	ASP	A	246	50.887	73.920	-0.656	1.00	34.38
3452	CA	ASP	A	246	49.489	73.995	-0.211	1.00	34.75
3454	CB	ASP	A	246	48.602	73.159	-1.151	1.00	35.30
3457	CG	ASP	A	246	47.185	73.699	-1.272	1.00	38.65
3458	OD1	ASP	A	246	46.738	73.925	-2.425	1.00	42.04
3459	OD2	ASP	A	246	46.433	73.914	-0.284	1.00	42.91
3460	C	ASP	A	246	49.431	73.410	1.198	1.00	33.97
3461	O	ASP	A	246	50.088	72.411	1.456	1.00	33.79
3462	N	THR	A	247	48.643	74.009	2.089	1.00	33.08
3464	CA	THR	A	247	48.489	73.517	3.465	1.00	32.87
3466	CB	THR	A	247	47.476	74.394	4.249	1.00	32.46
3468	OG1	THR	A	247	48.002	75.710	4.420	1.00	32.70
3470	CG2	THR	A	247	47.288	73.901	5.684	1.00	32.42
3474	C	THR	A	247	48.061	72.041	3.542	1.00	32.67
3475	O	THR	A	247	48.561	71.297	4.377	1.00	32.65
3476	N	ALA	A	248	47.141	71.617	2.677	1.00	32.34
3478	CA	ALA	A	248	46.651	70.240	2.709	1.00	32.14
3480	CB	ALA	A	248	45.388	70.095	1.857	1.00	32.51
3484	C	ALA	A	248	47.724	69.228	2.271	1.00	31.60
3485	O	ALA	A	248	47.692	68.073	2.678	1.00	31.38
3486	N	THR	A	249	48.668	69.666	1.447	1.00	31.12
3488	CA	THR	A	249	49.785	68.815	1.025	1.00	31.09
3490	CB	THR	A	249	50.269	69.251	-0.371	1.00	31.32
3492	OG1	THR	A	249	49.192	69.112	-1.313	1.00	33.79
3494	CG2	THR	A	249	51.348	68.308	-0.917	1.00	31.41
3498	C	THR	A	249	50.943	68.825	2.045	1.00	30.23
3499	O	THR	A	249	51.483	67.768	2.391	1.00	30.03
3500	N	LEU	A	250	51.312	70.017	2.520	1.00	29.30
3502	CA	LEU	A	250	52.358	70.175	3.539	1.00	28.64
3504	CB	LEU	A	250	52.668	71.653	3.766	1.00	28.31
3507	CG	LEU	A	250	53.253	72.412	2.577	1.00	29.19
3509	CD1	LEU	A	250	53.329	73.903	2.883	1.00	29.07
3513	CD2	LEU	A	250	54.620	71.880	2.197	1.00	29.56
3517	C	LEU	A	250	52.007	69.554	4.880	1.00	27.73
3518	O	LEU	A	250	52.877	69.038	5.578	1.00	27.92

FIGURE 3 ~~(Cont.)~~BI

A	B	C	D	E	F	G	H	I	J
3519	N	GLY	A	251	50.732	69.613	5.240	1.00	26.76
3521	CA	GLY	A	251	50.277	69.195	6.546	1.00	26.19
3524	C	GLY	A	251	50.485	70.266	7.601	1.00	25.80
3525	O	GLY	A	251	50.150	70.053	8.757	1.00	24.95
3526	N	LYS	A	252	51.071	71.388	7.197	1.00	25.86
3528	CA	LYS	A	252	51.273	72.556	8.052	1.00	26.53
3530	CB	LYS	A	252	52.701	72.588	8.628	1.00	25.80
3533	CG	LYS	A	252	53.804	72.498	7.579	1.00	25.64
3536	CD	LYS	A	252	55.183	72.231	8.200	1.00	23.61
3539	CE	LYS	A	252	56.297	72.507	7.205	1.00	22.86
3542	NZ	LYS	A	252	57.604	71.866	7.602	1.00	21.94
3546	C	LYS	A	252	50.992	73.813	7.223	1.00	27.55
3547	O	LYS	A	252	51.046	73.781	5.982	1.00	28.12
3548	N	ARG	A	253	50.721	74.918	7.905	1.00	28.61
3550	CA	ARG	A	253	50.217	76.128	7.249	1.00	29.63
3552	CB	ARG	A	253	49.658	77.096	8.287	1.00	30.10
3555	CG	ARG	A	253	48.370	76.612	8.875	1.00	32.12
3558	CD	ARG	A	253	47.441	77.693	9.362	1.00	35.28
3561	NE	ARG	A	253	46.380	77.104	10.175	1.00	38.07
3563	CZ	ARG	A	253	45.308	76.476	9.688	1.00	40.08
3564	NH1	ARG	A	253	45.095	76.378	8.376	1.00	39.60
3567	NH2	ARG	A	253	44.419	75.962	10.533	1.00	40.97
3570	C	ARG	A	253	51.223	76.852	6.360	1.00	29.71
3571	O	ARG	A	253	52.306	77.274	6.806	1.00	29.38
3572	N	GLN	A	254	50.847	76.966	5.084	1.00	30.10
3574	CA	GLN	A	254	51.544	77.794	4.108	1.00	29.94
3576	CB	GLN	A	254	50.816	77.731	2.754	1.00	30.17
3579	CG	GLN	A	254	51.436	78.643	1.649	1.00	31.83
3582	CD	GLN	A	254	50.618	78.716	0.357	1.00	34.25
3583	OE1	GLN	A	254	51.157	79.057	-0.705	1.00	35.57
3584	NE2	GLN	A	254	49.333	78.396	0.439	1.00	35.68
3587	C	GLN	A	254	51.586	79.238	4.601	1.00	29.79
3588	O	GLN	A	254	50.625	79.733	5.193	1.00	29.82
3589	N	GLY	A	255	52.705	79.907	4.369	1.00	29.23
3591	CA	GLY	A	255	52.843	81.298	4.740	1.00	29.36
3594	C	GLY	A	255	53.063	81.513	6.230	1.00	29.17
3595	O	GLY	A	255	52.963	82.630	6.708	1.00	28.41
3596	N	ALA	A	256	53.372	80.453	6.971	1.00	29.32
3598	CA	ALA	A	256	53.670	80.594	8.395	1.00	29.31
3600	CB	ALA	A	256	53.865	79.216	9.032	1.00	29.54
3604	C	ALA	A	256	54.900	81.481	8.638	1.00	29.48
3605	O	ALA	A	256	54.915	82.276	9.569	1.00	30.09
3606	N	ASP	A	257	55.925	81.350	7.805	1.00	29.41
3608	CA	ASP	A	257	57.170	82.079	8.006	1.00	29.43
3610	CB	ASP	A	257	58.242	81.581	7.053	1.00	29.35
3613	CG	ASP	A	257	58.770	80.208	7.420	1.00	28.93
3614	OD1	ASP	A	257	58.493	79.724	8.552	1.00	27.10
3615	OD2	ASP	A	257	59.480	79.562	6.613	1.00	25.07
3616	C	ASP	A	257	56.992	83.576	7.772	1.00	30.15
3617	O	ASP	A	257	57.516	84.404	8.505	1.00	28.74
3618	N	GLN	A	258	56.258	83.887	6.717	1.00	31.27
3620	CA	GLN	A	258	56.003	85.254	6.311	1.00	32.11

FIGURE 3 (Cont.)BJ

A	B	C	D	E	F	G	H	I	J
3622	CB	BGLN	A	258	55.223	85.271	4.997	0.35	32.00
3623	CB	AGLN	A	258	55.313	85.259	4.930	0.65	32.18
3628	CG	BGLN	A	258	55.115	86.632	4.342	0.35	31.76
3629	CG	AGLN	A	258	56.317	84.920	3.801	0.65	32.43
3634	CD	BGLN	A	258	54.771	86.519	2.876	0.35	31.23
3635	CD	AGLN	A	258	55.724	84.264	2.547	0.65	32.97
3636	OE1BGLN		A	258	55.645	86.639	2.016	0.35	30.93
3637	OE1AGLN		A	258	54.977	83.279	2.618	0.65	32.08
3638	NE2BGLN		A	258	53.503	86.266	2.585	0.35	30.18
3639	NE2AGLN		A	258	56.103	84.792	1.389	0.65	33.37
3644	C	GLN	A	258	55.203	85.967	7.400	1.00	32.82
3645	O	GLN	A	258	55.460	87.123	7.720	1.00	33.46
3646	N	GLN	A	259	54.266	85.249	8.000	1.00	33.70
3648	CA	GLN	A	259	53.452	85.780	9.084	1.00	34.64
3650	CB	GLN	A	259	52.395	84.756	9.463	1.00	35.35
3653	CG	GLN	A	259	51.346	85.257	10.436	1.00	38.57
3656	CD	GLN	A	259	50.161	84.331	10.482	1.00	42.61
3657	OE1	GLN	A	259	49.161	84.555	9.787	1.00	45.33
3658	NE2	GLN	A	259	50.272	83.263	11.278	1.00	44.63
3661	C	GLN	A	259	54.281	86.173	10.320	1.00	34.20
3662	O	GLN	A	259	53.948	87.154	10.990	1.00	33.93
3663	N	LEU	A	260	55.347	85.419	10.613	1.00	33.21
3665	CA	LEU	A	260	56.247	85.737	11.734	1.00	32.74
3667	CB	LEU	A	260	56.676	84.463	12.474	1.00	32.73
3670	CG	LEU	A	260	55.629	83.549	13.112	1.00	34.09
3672	CD1	LEU	A	260	56.300	82.734	14.206	1.00	35.07
3676	CD2	LEU	A	260	54.412	84.295	13.676	1.00	35.20
3680	C	LEU	A	260	57.514	86.495	11.326	1.00	31.74
3681	O	LEU	A	260	58.348	86.790	12.172	1.00	31.90
3682	N	GLY	A	261	57.670	86.808	10.043	1.00	30.66
3684	CA	GLY	A	261	58.858	87.495	9.565	1.00	29.51
3687	C	GLY	A	261	60.157	86.732	9.759	1.00	28.74
3688	O	GLY	A	261	61.198	87.333	9.998	1.00	28.52
3689	N	LYS	A	262	60.099	85.405	9.649	1.00	27.62
3691	CA	LYS	A	262	61.296	84.575	9.707	1.00	26.77
3693	CB	LYS	A	262	60.934	83.092	9.572	1.00	26.29
3696	CG	LYS	A	262	60.021	82.536	10.642	1.00	25.90
3699	CD	LYS	A	262	60.797	82.141	11.884	1.00	26.17
3702	CE	LYS	A	262	59.882	81.593	12.965	1.00	26.68
3705	NZ	LYS	A	262	60.644	81.319	14.214	1.00	25.74
3709	C	LYS	A	262	62.280	84.943	8.595	1.00	26.39
3710	O	LYS	A	262	61.884	85.161	7.445	1.00	26.03
3711	N	SER	A	263	63.563	85.005	8.943	1.00	26.23
3713	CA	SER	A	263	64.629	85.019	7.944	1.00	26.10
3715	CB	SER	A	263	65.975	85.311	8.586	1.00	26.43
3718	OG	SER	A	263	65.979	86.581	9.207	1.00	26.96
3720	C	SER	A	263	64.666	83.652	7.247	1.00	26.21
3721	O	SER	A	263	64.899	82.629	7.898	1.00	25.19
3722	N	THR	A	264	64.388	83.642	5.942	1.00	25.65
3724	CA	THR	A	264	64.408	82.408	5.149	1.00	25.89
3726	CB	THR	A	264	62.975	81.922	4.812	1.00	26.14
3728	OG1	THR	A	264	62.368	82.789	3.847	1.00	26.91

FIGURE 3 ~~(Cont.)~~BK

A	B	C	D	E	F	G	H	I	J
3730	CG2	THR	A	264	62.046	81.992	6.033	1.00	26.45
3734	C	THR	A	264	65.189	82.591	3.856	1.00	25.77
3735	O	THR	A	264	65.538	83.722	3.472	1.00	25.52
3736	N	TYR	A	265	65.479	81.471	3.195	1.00	25.31
3738	CA	TYR	A	265	66.114	81.507	1.886	1.00	25.24
3740	CB	TYR	A	265	66.555	80.104	1.428	1.00	24.84
3743	CG	TYR	A	265	67.953	79.767	1.902	1.00	24.29
3744	CD1	TYR	A	265	69.012	79.698	1.010	1.00	23.63
3746	CE1	TYR	A	265	70.282	79.407	1.423	1.00	24.04
3748	CZ	TYR	A	265	70.545	79.200	2.759	1.00	24.29
3749	OH	TYR	A	265	71.827	78.928	3.168	1.00	24.41
3751	CE2	TYR	A	265	69.521	79.276	3.685	1.00	24.92
3753	CD2	TYR	A	265	68.225	79.566	3.250	1.00	23.77
3755	C	TYR	A	265	65.240	82.222	0.843	1.00	25.25
3756	O	TYR	A	265	65.717	83.149	0.211	1.00	25.83
3757	N	PRO	A	266	63.982	81.823	0.658	1.00	25.61
3758	CA	PRO	A	266	63.108	82.515	-0.307	1.00	25.70
3760	CB	PRO	A	266	61.812	81.700	-0.284	1.00	26.04
3763	CG	PRO	A	266	61.876	80.854	0.923	1.00	26.04
3766	CD	PRO	A	266	63.311	80.683	1.293	1.00	25.37
3769	C	PRO	A	266	62.825	83.980	0.027	1.00	25.95
3770	O	PRO	A	266	62.702	84.784	-0.900	1.00	25.00
3771	N	ALA	A	267	62.738	84.326	1.311	1.00	26.04
3773	CA	ALA	A	267	62.503	85.719	1.697	1.00	26.33
3775	CB	ALA	A	267	62.193	85.853	3.166	1.00	26.37
3779	C	ALA	A	267	63.694	86.578	1.309	1.00	26.47
3780	O	ALA	A	267	63.512	87.637	0.734	1.00	26.90
3781	N	LEU	A	268	64.906	86.094	1.574	1.00	26.35
3783	CA	LEU	A	268	66.124	86.814	1.213	1.00	26.27
3785	CB	LEU	A	268	67.337	86.201	1.924	1.00	26.30
3788	CG	LEU	A	268	68.691	86.873	1.690	1.00	27.65
3790	CD1	LEU	A	268	68.728	88.322	2.211	1.00	28.07
3794	CD2	LEU	A	268	69.803	86.053	2.316	1.00	28.26
3798	C	LEU	A	268	66.386	86.828	-0.294	1.00	26.01
3799	O	LEU	A	268	66.541	87.899	-0.898	1.00	25.44
3800	N	LEU	A	269	66.439	85.633	-0.881	1.00	25.58
3802	CA	LEU	A	269	66.963	85.430	-2.234	1.00	25.43
3804	CB	LEU	A	269	67.755	84.113	-2.298	1.00	25.44
3807	CG	LEU	A	269	68.906	83.896	-1.320	1.00	26.67
3809	CD1	LEU	A	269	69.520	82.486	-1.510	1.00	25.96
3813	CD2	LEU	A	269	69.960	84.976	-1.479	1.00	27.24
3817	C	LEU	A	269	65.902	85.380	-3.316	1.00	24.91
3818	O	LEU	A	269	66.226	85.454	-4.490	1.00	24.92
3819	N	GLY	A	270	64.640	85.253	-2.933	1.00	24.87
3821	CA	GLY	A	270	63.584	84.945	-3.884	1.00	24.94
3824	C	GLY	A	270	63.529	83.446	-4.151	1.00	25.33
3825	O	GLY	A	270	64.488	82.724	-3.871	1.00	25.08
3826	N	LEU	A	271	62.415	82.985	-4.699	1.00	25.79
3828	CA	LEU	A	271	62.170	81.567	-4.899	1.00	26.67
3830	CB	LEU	A	271	60.732	81.320	-5.383	1.00	27.35
3833	CG	LEU	A	271	59.602	81.477	-4.365	1.00	28.42
3835	CD1	LEU	A	271	58.252	81.403	-5.068	1.00	29.93

FIGURE 3 ~~(Cont.)~~BL

A	B	C	D	E	F	G	H	I	J
3839	CD2	LEU	A	271	59.687	80.413	-3.279	1.00	28.63
3843	C	LEU	A	271	63.162	80.914	-5.853	1.00	27.13
3844	O	LEU	A	271	63.593	79.796	-5.591	1.00	27.11
3845	N	GLU	A	272	63.536	81.599	-6.938	1.00	27.48
3847	CA	GLU	A	272	64.429	81.018	-7.956	1.00	28.05
3849	CB	GLU	A	272	64.488	81.905	-9.229	1.00	28.98
3852	CG	GLU	A	272	65.687	81.611	-10.148	1.00	31.69
3855	CD	GLU	A	272	65.592	82.253	-11.528	1.00	35.38
3856	OE1	GLU	A	272	66.103	81.648	-12.499	1.00	39.00
3857	OE2	GLU	A	272	65.013	83.354	-11.655	1.00	37.35
3858	C	GLU	A	272	65.850	80.739	-7.455	1.00	27.43
3859	O	GLU	A	272	66.427	79.668	-7.745	1.00	27.14
3860	N	GLN	A	273	66.432	81.697	-6.743	1.00	26.16
3862	CA	GLN	A	273	67.799	81.563	-6.250	1.00	26.17
3864	CB	GLN	A	273	68.364	82.909	-5.793	1.00	26.14
3867	CG	GLN	A	273	68.642	83.881	-6.920	1.00	29.26
3870	CD	GLN	A	273	69.025	85.266	-6.418	1.00	32.23
3871	OE1	GLN	A	273	69.828	85.405	-5.485	1.00	34.54
3872	NE2	GLN	A	273	68.464	86.295	-7.046	1.00	34.59
3875	C	GLN	A	273	67.854	80.566	-5.092	1.00	25.40
3876	O	GLN	A	273	68.856	79.905	-4.900	1.00	25.15
3877	N	ALA	A	274	66.776	80.485	-4.318	1.00	25.33
3879	CA	ALA	A	274	66.681	79.514	-3.239	1.00	25.32
3881	CB	ALA	A	274	65.429	79.770	-2.427	1.00	25.59
3885	C	ALA	A	274	66.665	78.097	-3.837	1.00	25.68
3886	O	ALA	A	274	67.388	77.213	-3.385	1.00	25.35
3887	N	ARG	A	275	65.860	77.913	-4.878	1.00	25.78
3889	CA	ARG	A	275	65.753	76.631	-5.564	1.00	26.49
3891	CB	ARG	A	275	64.725	76.697	-6.683	1.00	26.59
3894	CG	ARG	A	275	63.311	76.604	-6.197	1.00	27.19
3897	CD	ARG	A	275	62.284	76.791	-7.294	1.00	29.91
3900	NE	ARG	A	275	60.926	76.575	-6.799	1.00	31.85
3902	CZ	ARG	A	275	59.886	77.379	-7.009	1.00	34.22
3903	NH1	ARG	A	275	59.998	78.504	-7.720	1.00	35.16
3906	NH2	ARG	A	275	58.706	77.047	-6.491	1.00	35.99
3909	C	ARG	A	275	67.091	76.201	-6.109	1.00	26.94
3910	O	ARG	A	275	67.468	75.039	-5.985	1.00	27.03
3911	N	LYS	A	276	67.816	77.155	-6.679	1.00	27.58
3913	CA	LYS	A	276	69.145	76.929	-7.218	1.00	28.35
3915	CB	LYS	A	276	69.641	78.193	-7.934	1.00	29.25
3918	CG	LYS	A	276	71.101	78.163	-8.408	1.00	31.10
3921	CD	LYS	A	276	71.288	77.283	-9.637	1.00	34.04
3924	CE	LYS	A	276	72.514	77.689	-10.473	1.00	35.05
3927	NZ	LYS	A	276	73.803	77.493	-9.748	1.00	35.48
3931	C	LYS	A	276	70.130	76.552	-6.132	1.00	28.37
3932	O	LYS	A	276	70.987	75.692	-6.347	1.00	28.80
3933	N	LYS	A	277	70.054	77.222	-4.986	1.00	28.08
3935	CA	LYS	A	277	70.938	76.890	-3.873	1.00	27.92
3937	CB	LYS	A	277	70.723	77.824	-2.675	1.00	28.22
3940	CG	LYS	A	277	71.163	79.279	-2.921	1.00	30.08
3943	CD	LYS	A	277	72.546	79.581	-2.376	1.00	31.98
3946	CE	LYS	A	277	72.871	81.085	-2.414	1.00	32.86

FIGURE 3 ~~(Cont.)~~BM

A	B	C	D	E	F	G	H	I	J
3949	NZ	LYS	A	277	74.277	81.323	-2.846	1.00	33.80
3953	C	LYS	A	277	70.680	75.438	-3.453	1.00	27.24
3954	O	LYS	A	277	71.620	74.699	-3.201	1.00	26.52
3955	N	ALA	A	278	69.411	75.041	-3.393	1.00	26.71
3957	CA	ALA	A	278	69.053	73.682	-2.960	1.00	26.99
3959	CB	ALA	A	278	67.544	73.546	-2.823	1.00	26.84
3963	C	ALA	A	278	69.589	72.651	-3.949	1.00	27.26
3964	O	ALA	A	278	70.141	71.636	-3.566	1.00	26.69
3965	N	ARG	A	279	69.427	72.948	-5.234	1.00	27.61
3967	CA	ARG	A	279	69.869	72.070	-6.311	1.00	28.16
3969	CB	ARG	A	279	69.332	72.603	-7.641	1.00	28.87
3972	CG	ARG	A	279	69.910	71.996	-8.886	1.00	32.19
3975	CD	ARG	A	279	69.160	72.414	-10.158	1.00	35.33
3978	NE	ARG	A	279	68.039	73.319	-9.871	1.00	38.00
3980	CZ	ARG	A	279	68.005	74.632	-10.133	1.00	38.95
3981	NH1	ARG	A	279	69.027	75.256	-10.711	1.00	40.27
3984	NH2	ARG	A	279	66.924	75.329	-9.815	1.00	38.71
3987	C	ARG	A	279	71.389	71.923	-6.336	1.00	27.24
3988	O	ARG	A	279	71.885	70.819	-6.512	1.00	27.02
3989	N	ASP	A	280	72.116	73.021	-6.128	1.00	26.36
3991	CA	ASP	A	280	73.586	72.995	-6.059	1.00	25.90
3993	CB	ASP	A	280	74.150	74.420	-6.005	1.00	26.39
3996	CG	ASP	A	280	74.006	75.175	-7.335	1.00	28.03
3997	OD1	ASP	A	280	74.090	76.423	-7.315	1.00	30.25
3998	OD2	ASP	A	280	73.790	74.623	-8.433	1.00	28.83
3999	C	ASP	A	280	74.086	72.217	-4.828	1.00	25.37
4000	O	ASP	A	280	75.128	71.557	-4.873	1.00	24.74
4001	N	LEU	A	281	73.346	72.307	-3.727	1.00	24.45
4003	CA	LEU	A	281	73.688	71.553	-2.529	1.00	24.47
4005	CB	LEU	A	281	72.825	71.999	-1.335	1.00	24.55
4008	CG	LEU	A	281	73.246	73.324	-0.700	1.00	23.94
4010	CD1	LEU	A	281	72.129	73.904	0.129	1.00	23.80
4014	CD2	LEU	A	281	74.506	73.133	0.150	1.00	23.78
4018	C	LEU	A	281	73.526	70.048	-2.781	1.00	24.25
4019	O	LEU	A	281	74.364	69.262	-2.353	1.00	23.54
4020	N	ILE	A	282	72.459	69.660	-3.475	1.00	24.75
4022	CA	ILE	A	282	72.221	68.242	-3.788	1.00	25.66
4024	CB	ILE	A	282	70.771	67.998	-4.289	1.00	25.32
4026	CG1	ILE	A	282	69.745	68.291	-3.185	1.00	25.41
4029	CD1	ILE	A	282	70.153	67.917	-1.800	1.00	25.34
4033	CG2	ILE	A	282	70.592	66.548	-4.826	1.00	25.27
4037	C	ILE	A	282	73.241	67.719	-4.788	1.00	26.42
4038	O	ILE	A	282	73.728	66.602	-4.641	1.00	26.98
4039	N	ASP	A	283	73.571	68.511	-5.802	1.00	27.38
4041	CA	ASP	A	283	74.607	68.111	-6.753	1.00	28.16
4043	CB	ASP	A	283	74.799	69.165	-7.851	1.00	28.99
4046	CG	ASP	A	283	73.578	69.319	-8.758	1.00	31.72
4047	OD1	ASP	A	283	73.510	70.341	-9.477	1.00	36.96
4048	OD2	ASP	A	283	72.644	68.493	-8.830	1.00	35.17
4049	C	ASP	A	283	75.929	67.903	-5.997	1.00	27.86
4050	O	ASP	A	283	76.696	67.003	-6.319	1.00	27.48
4051	N	ASP	A	284	76.189	68.740	-4.988	1.00	27.56

FIGURE 3 ~~(Cont.)~~BN

A	B	C	D	E	F	G	H	I	J
4053	CA	ASP	A	284	77.405	68.623	-4.177	1.00	27.43
4055	CB	ASP	A	284	77.573	69.869	-3.296	1.00	27.98
4058	CG	ASP	A	284	78.753	69.774	-2.351	1.00	29.55
4059	OD1	ASP	A	284	79.871	70.166	-2.754	1.00	34.48
4060	OD2	ASP	A	284	78.662	69.347	-1.179	1.00	30.96
4061	C	ASP	A	284	77.344	67.351	-3.320	1.00	26.91
4062	O	ASP	A	284	78.347	66.666	-3.137	1.00	26.70
4063	N	ALA	A	285	76.154	67.039	-2.817	1.00	26.35
4065	CA	ALA	A	285	75.935	65.830	-2.041	1.00	26.26
4067	CB	ALA	A	285	74.514	65.811	-1.452	1.00	26.18
4071	C	ALA	A	285	76.164	64.607	-2.913	1.00	26.41
4072	O	ALA	A	285	76.774	63.648	-2.469	1.00	26.46
4073	N	ARG	A	286	75.687	64.647	-4.156	1.00	26.93
4075	CA	ARG	A	286	75.888	63.543	-5.095	1.00	27.77
4077	CB	ARG	A	286	75.153	63.778	-6.413	1.00	28.06
4080	CG	ARG	A	286	73.650	63.500	-6.353	1.00	30.42
4083	CD	ARG	A	286	72.949	63.511	-7.727	1.00	33.16
4086	NE	ARG	A	286	71.739	62.694	-7.695	1.00	35.04
4088	CZ	ARG	A	286	71.709	61.365	-7.828	1.00	37.56
4089	NH1	ARG	A	286	72.820	60.653	-8.041	1.00	37.77
4092	NH2	ARG	A	286	70.544	60.731	-7.757	1.00	37.95
4095	C	ARG	A	286	77.377	63.333	-5.364	1.00	28.02
4096	O	ARG	A	286	77.837	62.202	-5.438	1.00	27.64
4097	N	GLN	A	287	78.120	64.427	-5.478	1.00	28.41
4099	CA	GLN	A	287	79.550	64.352	-5.768	1.00	29.05
4101	CB	GLN	A	287	80.163	65.742	-5.984	1.00	29.26
4104	CG	GLN	A	287	79.870	66.348	-7.343	1.00	31.16
4107	CD	GLN	A	287	80.342	65.469	-8.494	1.00	34.10
4108	OE1	GLN	A	287	81.544	65.280	-8.687	1.00	36.57
4109	NE2	GLN	A	287	79.396	64.921	-9.248	1.00	34.65
4112	C	GLN	A	287	80.260	63.638	-4.645	1.00	28.84
4113	O	GLN	A	287	81.060	62.747	-4.898	1.00	29.43
4114	N	SER	A	288	79.946	64.002	-3.403	1.00	28.72
4116	CA	SER	A	288	80.514	63.331	-2.234	1.00	28.70
4118	CB	SER	A	288	79.948	63.912	-0.930	1.00	28.50
4121	OG	SER	A	288	80.451	65.214	-0.693	1.00	28.19
4123	C	SER	A	288	80.254	61.824	-2.255	1.00	28.86
4124	O	SER	A	288	81.143	61.046	-1.948	1.00	28.79
4125	N	LEU	A	289	79.028	61.428	-2.579	1.00	29.44
4127	CA	LEU	A	289	78.666	60.005	-2.650	1.00	29.79
4129	CB	LEU	A	289	77.163	59.818	-2.910	1.00	29.50
4132	CG	LEU	A	289	76.184	60.273	-1.815	1.00	28.59
4134	CD1	LEU	A	289	74.747	60.026	-2.249	1.00	28.94
4138	CD2	LEU	A	289	76.473	59.585	-0.493	1.00	27.92
4142	C	LEU	A	289	79.472	59.246	-3.717	1.00	30.81
4143	O	LEU	A	289	79.732	58.062	-3.545	1.00	30.71
4144	N	LYS	A	290	79.870	59.919	-4.800	1.00	31.59
4146	CA	LYS	A	290	80.704	59.288	-5.837	1.00	32.26
4148	CB	LYS	A	290	80.998	60.268	-6.989	1.00	32.55
4151	CG	LYS	A	290	79.794	60.560	-7.898	1.00	34.13
4154	CD	LYS	A	290	80.188	61.386	-9.153	1.00	35.23
4157	CE	LYS	A	290	79.129	61.238	-10.259	1.00	36.81

FIGURE 3 ~~(Cont.)~~BO

A	B	C	D	E	F	G	H	I	J
4160	NZ	LYS	A	290	79.083	62.387	-11.229	1.00	37.86
4164	C	LYS	A	290	82.012	58.741	-5.256	1.00	32.60
4165	O	LYS	A	290	82.471	57.679	-5.650	1.00	33.03
4166	N	GLN	A	291	82.589	59.462	-4.300	1.00	33.38
4168	CA	GLN	A	291	83.796	59.026	-3.599	1.00	34.01
4170	CB	GLN	A	291	84.253	60.103	-2.607	1.00	34.60
4173	CG	GLN	A	291	84.614	61.448	-3.230	1.00	35.87
4176	CD	GLN	A	291	85.108	62.446	-2.197	1.00	37.47
4177	OE1	GLN	A	291	86.039	62.155	-1.446	1.00	39.36
4178	NE2	GLN	A	291	84.483	63.615	-2.149	1.00	39.06
4181	C	GLN	A	291	83.589	57.715	-2.830	1.00	34.18
4182	O	GLN	A	291	84.513	56.909	-2.707	1.00	34.15
4183	N	LEU	A	292	82.385	57.520	-2.294	1.00	33.99
4185	CA	LEU	A	292	82.047	56.287	-1.591	1.00	34.26
4187	CB	LEU	A	292	80.849	56.509	-0.670	1.00	33.95
4190	CG	LEU	A	292	81.061	57.578	0.398	1.00	33.40
4192	CD1	LEU	A	292	79.805	57.720	1.223	1.00	33.09
4196	CD2	LEU	A	292	82.269	57.242	1.274	1.00	33.91
4200	C	LEU	A	292	81.738	55.137	-2.533	1.00	34.79
4201	O	LEU	A	292	82.073	53.989	-2.239	1.00	34.64
4202	N	ALA	A	293	81.072	55.445	-3.642	1.00	35.56
4204	CA	ALA	A	293	80.741	54.450	-4.660	1.00	36.49
4206	CB	ALA	A	293	79.825	55.061	-5.712	1.00	36.38
4210	C	ALA	A	293	82.012	53.886	-5.311	1.00	37.32
4211	O	ALA	A	293	82.015	52.758	-5.799	1.00	37.70
4212	N	GLU	A	294	83.075	54.690	-5.296	1.00	38.52
4214	CA	GLU	A	294	84.421	54.297	-5.744	1.00	39.54
4216	CB	GLU	A	294	85.353	55.513	-5.677	1.00	39.78
4219	CG	GLU	A	294	86.404	55.572	-6.767	1.00	41.97
4222	CD	GLU	A	294	86.407	56.897	-7.488	1.00	43.76
4223	OE1	GLU	A	294	86.681	57.915	-6.825	1.00	46.66
4224	OE2	GLU	A	294	86.129	56.921	-8.705	1.00	45.53
4225	C	GLU	A	294	85.034	53.179	-4.895	1.00	39.49
4226	O	GLU	A	294	85.883	52.422	-5.363	1.00	40.00
4227	N	GLN	A	295	84.617	53.112	-3.638	1.00	39.43
4229	CA	GLN	A	295	85.085	52.109	-2.700	1.00	39.30
4231	CB	GLN	A	295	85.306	52.752	-1.324	1.00	39.51
4234	CG	GLN	A	295	86.094	54.061	-1.348	1.00	40.85
4237	CD	GLN	A	295	86.003	54.825	-0.033	1.00	42.68
4238	OE1	GLN	A	295	85.958	54.217	1.037	1.00	44.83
4239	NE2	GLN	A	295	85.983	56.156	-0.110	1.00	42.30
4242	C	GLN	A	295	84.087	50.944	-2.594	1.00	38.62
4243	O	GLN	A	295	84.083	50.210	-1.605	1.00	38.99
4244	N	SER	A	296	83.250	50.794	-3.616	1.00	37.61
4246	CA	SER	A	296	82.260	49.718	-3.721	1.00	36.98
4248	CB	SER	A	296	82.963	48.362	-3.884	1.00	37.17
4251	OG	SER	A	296	83.487	48.241	-5.197	1.00	38.77
4253	C	SER	A	296	81.210	49.685	-2.598	1.00	35.68
4254	O	SER	A	296	80.722	48.617	-2.206	1.00	35.55
4255	N	LEU	A	297	80.867	50.865	-2.092	1.00	34.25
4257	CA	LEU	A	297	79.710	51.032	-1.218	1.00	32.88
4259	CB	LEU	A	297	79.997	52.090	-0.161	1.00	32.92

FIGURE 3 ~~(Cont.)~~BP

A	B	C	D	E	F	G	H	I	J
4262	CG	LEU	A	297	81.178	51.793	0.755	1.00	33.21
4264	CD1	LEU	A	297	81.567	53.040	1.532	1.00	33.05
4268	CD2	LEU	A	297	80.872	50.609	1.704	1.00	33.61
4272	C	LEU	A	297	78.507	51.432	-2.074	1.00	31.66
4273	O	LEU	A	297	78.621	52.255	-2.988	1.00	31.32
4274	N	ASP	A	298	77.361	50.827	-1.799	1.00	30.63
4276	CA	ASP	A	298	76.127	51.123	-2.528	1.00	29.60
4278	CB	ASP	A	298	75.150	49.956	-2.371	1.00	29.83
4281	CG	ASP	A	298	73.911	50.089	-3.251	1.00	30.98
4282	OD1	ASP	A	298	73.673	51.177	-3.843	1.00	30.78
4283	OD2	ASP	A	298	73.117	49.135	-3.407	1.00	32.78
4284	C	ASP	A	298	75.516	52.431	-2.021	1.00	28.62
4285	O	ASP	A	298	74.919	52.474	-0.953	1.00	27.93
4286	N	THR	A	299	75.655	53.496	-2.801	1.00	27.78
4288	CA	THR	A	299	75.152	54.812	-2.395	1.00	27.48
4290	CB	THR	A	299	76.121	55.907	-2.850	1.00	27.79
4292	OG1	THR	A	299	76.198	55.923	-4.282	1.00	27.64
4294	CG2	THR	A	299	77.522	55.612	-2.397	1.00	27.86
4298	C	THR	A	299	73.775	55.130	-2.963	1.00	26.98
4299	O	THR	A	299	73.314	56.269	-2.852	1.00	26.90
4300	N	SER	A	300	73.115	54.136	-3.549	1.00	25.87
4302	CA	SER	A	300	71.884	54.371	-4.303	1.00	25.78
4304	CB	SER	A	300	71.469	53.116	-5.083	1.00	25.66
4307	OG	SER	A	300	71.181	52.042	-4.210	1.00	28.03
4309	C	SER	A	300	70.718	54.922	-3.460	1.00	24.86
4310	O	SER	A	300	69.989	55.799	-3.922	1.00	24.04
4311	N	ALA	A	301	70.538	54.423	-2.237	1.00	24.31
4313	CA	ALA	A	301	69.491	54.957	-1.356	1.00	23.85
4315	CB	ALA	A	301	69.266	54.058	-0.138	1.00	23.74
4319	C	ALA	A	301	69.813	56.402	-0.925	1.00	23.51
4320	O	ALA	A	301	68.927	57.234	-0.865	1.00	22.49
4321	N	LEU	A	302	71.082	56.696	-0.670	1.00	23.59
4323	CA	LEU	A	302	71.476	58.050	-0.254	1.00	24.04
4325	CB	LEU	A	302	72.893	58.059	0.321	1.00	23.68
4328	CG	LEU	A	302	73.047	57.380	1.677	1.00	24.07
4330	CD1	LEU	A	302	74.495	57.511	2.165	1.00	25.59
4334	CD2	LEU	A	302	72.085	57.972	2.680	1.00	24.26
4338	C	LEU	A	302	71.375	59.070	-1.370	1.00	24.05
4339	O	LEU	A	302	71.128	60.238	-1.104	1.00	24.30
4340	N	GLU	A	303	71.575	58.648	-2.614	1.00	24.92
4342	CA	GLU	A	303	71.455	59.578	-3.734	1.00	25.79
4344	CB	GLU	A	303	72.238	59.158	-4.988	1.00	26.38
4347	CG	GLU	A	303	72.152	57.732	-5.448	1.00	28.99
4350	CD	GLU	A	303	73.344	57.345	-6.333	1.00	31.29
4351	OE1	GLU	A	303	73.673	58.127	-7.247	1.00	31.21
4352	OE2	GLU	A	303	73.966	56.274	-6.098	1.00	33.39
4353	C	GLU	A	303	69.982	59.834	-4.045	1.00	25.52
4354	O	GLU	A	303	69.605	60.961	-4.347	1.00	25.13
4355	N	ALA	A	304	69.152	58.797	-3.927	1.00	25.73
4357	CA	ALA	A	304	67.709	58.953	-4.149	1.00	25.33
4359	CB	ALA	A	304	67.020	57.609	-4.201	1.00	25.75
4363	C	ALA	A	304	67.099	59.830	-3.059	1.00	25.32

FIGURE 3 (Cont.)BQ

A	B	C	D	E	F	G	H	I	J
4364	O	ALA	A	304	66.202	60.633	-3.328	1.00	24.76
4365	N	LEU	A	305	67.591	59.677	-1.828	1.00	25.18
4367	CA	LEU	A	305	67.117	60.499	-0.711	1.00	25.23
4369	CB	LEU	A	305	67.707	59.988	0.608	1.00	25.28
4372	CG	LEU	A	305	67.209	60.548	1.945	1.00	27.23
4374	CD1	LEU	A	305	67.788	61.919	2.199	1.00	29.43
4378	CD2	LEU	A	305	65.687	60.595	2.012	1.00	28.69
4382	C	LEU	A	305	67.520	61.954	-0.959	1.00	24.32
4383	O	LEU	A	305	66.719	62.872	-0.780	1.00	23.70
4384	N	ALA	A	306	68.758	62.146	-1.399	1.00	23.80
4386	CA	ALA	A	306	69.282	63.481	-1.672	1.00	24.14
4388	CB	ALA	A	306	70.733	63.405	-2.153	1.00	24.17
4392	C	ALA	A	306	68.410	64.218	-2.687	1.00	24.07
4393	O	ALA	A	306	68.063	65.382	-2.480	1.00	23.69
4394	N	ASP	A	307	68.027	63.538	-3.761	1.00	24.24
4396	CA	ASP	A	307	67.146	64.143	-4.772	1.00	24.99
4398	CB	ASP	A	307	67.015	63.231	-5.990	1.00	25.46
4401	CG	ASP	A	307	68.259	63.225	-6.840	1.00	27.73
4402	OD1	ASP	A	307	68.311	62.445	-7.819	1.00	32.11
4403	OD2	ASP	A	307	69.231	63.968	-6.614	1.00	30.06
4404	C	ASP	A	307	65.751	64.427	-4.242	1.00	24.15
4405	O	ASP	A	307	65.146	65.464	-4.565	1.00	23.53
4406	N	TYR	A	308	65.233	63.497	-3.445	1.00	23.64
4408	CA	TYR	A	308	63.890	63.636	-2.889	1.00	23.49
4410	CB	TYR	A	308	63.465	62.369	-2.150	1.00	23.53
4413	CG	TYR	A	308	62.066	62.432	-1.543	1.00	23.83
4414	CD1	TYR	A	308	61.882	62.358	-0.171	1.00	24.83
4416	CE1	TYR	A	308	60.607	62.425	0.392	1.00	25.12
4418	CZ	TYR	A	308	59.501	62.553	-0.424	1.00	26.00
4419	OH	TYR	A	308	58.239	62.602	0.134	1.00	26.70
4421	CE2	TYR	A	308	59.660	62.622	-1.798	1.00	25.30
4423	CD2	TYR	A	308	60.939	62.568	-2.344	1.00	23.99
4425	C	TYR	A	308	63.824	64.844	-1.957	1.00	23.57
4426	O	TYR	A	308	62.829	65.529	-1.919	1.00	22.72
4427	N	ILE	A	309	64.902	65.112	-1.229	1.00	24.12
4429	CA	ILE	A	309	64.949	66.247	-0.301	1.00	24.93
4431	CB	ILE	A	309	66.333	66.304	0.411	1.00	24.90
4433	CG1	ILE	A	309	66.333	65.285	1.553	1.00	25.34
4436	CD1	ILE	A	309	67.675	65.077	2.197	1.00	27.41
4440	CG2	ILE	A	309	66.639	67.710	0.943	1.00	25.11
4444	C	ILE	A	309	64.575	67.576	-0.977	1.00	25.41
4445	O	ILE	A	309	64.017	68.468	-0.326	1.00	25.21
4446	N	ILE	A	310	64.848	67.702	-2.274	1.00	25.98
4448	CA	ILE	A	310	64.481	68.928	-3.003	1.00	26.46
4450	CB	ILE	A	310	65.736	69.586	-3.590	1.00	26.50
4452	CG1	ILE	A	310	66.349	68.722	-4.700	1.00	26.76
4455	CD1	ILE	A	310	67.350	69.472	-5.530	1.00	27.27
4459	CG2	ILE	A	310	66.729	69.819	-2.491	1.00	26.11
4463	C	ILE	A	310	63.393	68.781	-4.066	1.00	26.91
4464	O	ILE	A	310	62.930	69.779	-4.622	1.00	26.80
4465	N	GLN	A	311	62.982	67.543	-4.337	1.00	26.94
4467	CA	GLN	A	311	61.911	67.267	-5.284	1.00	27.25

FIGURE 3 ~~(Cont.)~~BR

A	B	C	D	E	F	G	H	I	J
4469	CB	GLN	A	311	62.217	65.999	-6.089	1.00	27.44
4472	CG	GLN	A	311	63.241	66.219	-7.186	1.00	30.05
4475	CD	GLN	A	311	63.720	64.922	-7.830	1.00	33.37
4476	OE1	GLN	A	311	64.730	64.920	-8.521	1.00	36.33
4477	NE2	GLN	A	311	62.999	63.828	-7.606	1.00	34.01
4480	C	GLN	A	311	60.573	67.102	-4.575	1.00	26.71
4481	O	GLN	A	311	59.514	67.225	-5.193	1.00	27.01
4482	N	ARG	A	312	60.620	66.825	-3.280	1.00	26.09
4484	CA	ARG	A	312	59.418	66.570	-2.503	1.00	25.94
4486	CB	ARG	A	312	59.774	66.077	-1.098	1.00	25.87
4489	CG	ARG	A	312	60.382	67.160	-0.225	1.00	25.06
4492	CD	ARG	A	312	61.211	66.630	0.914	1.00	23.99
4495	NE	ARG	A	312	61.963	67.704	1.555	1.00	22.64
4497	CZ	ARG	A	312	61.503	68.481	2.528	1.00	19.61
4498	NH1	ARG	A	312	62.286	69.429	3.025	1.00	20.15
4501	NH2	ARG	A	312	60.289	68.325	3.008	1.00	19.15
4504	C	ARG	A	312	58.558	67.817	-2.386	1.00	26.24
4505	O	ARG	A	312	59.053	68.938	-2.448	1.00	25.48
4506	N	ASN	A	313	57.269	67.601	-2.191	1.00	26.97
4508	CA	ASN	A	313	56.321	68.702	-2.054	1.00	28.44
4510	CB	ASN	A	313	55.255	68.594	-3.128	1.00	28.90
4513	CG	ASN	A	313	55.820	68.829	-4.487	1.00	31.25
4514	OD1	ASN	A	313	56.328	69.921	-4.771	1.00	36.72
4515	ND2	ASN	A	313	55.782	67.807	-5.337	1.00	35.16
4518	C	ASN	A	313	55.711	68.729	-0.676	1.00	28.47
4519	O	ASN	A	313	54.731	69.426	-0.440	1.00	28.00
4520	N	LYS	A	314	56.326	67.972	0.234	1.00	29.44
4522	CA	LYS	A	314	55.925	67.944	1.642	1.00	30.19
4524	CB	LYS	A	314	54.722	67.029	1.835	1.00	30.27
4527	CG	LYS	A	314	54.874	65.638	1.202	1.00	32.14
4530	CD	LYS	A	314	54.635	64.498	2.180	1.00	34.17
4533	CE	LYS	A	314	53.660	63.459	1.652	1.00	35.54
4536	NZ	LYS	A	314	54.228	62.656	0.542	1.00	36.19
4540	C	LYS	A	314	57.081	67.487	2.528	1.00	30.38
4541	O	LYS	A	314	56.992	67.504	3.759	1.00	30.94
4542	OXT	LYS	A	314	58.130	67.081	2.028	1.00	30.00
4543	N	ASP	B	17	19.060	6.498	-16.010	1.00	36.37
4545	CA	ASP	B	17	17.827	7.340	-15.968	1.00	36.07
4547	CB	ASP	B	17	16.585	6.454	-15.910	1.00	36.75
4550	CG	ASP	B	17	15.301	7.258	-15.889	1.00	38.21
4551	OD1	ASP	B	17	15.288	8.356	-16.476	1.00	42.09
4552	OD2	ASP	B	17	14.258	6.882	-15.321	1.00	41.73
4553	C	ASP	B	17	17.853	8.266	-14.742	1.00	35.62
4554	O	ASP	B	17	17.713	7.800	-13.603	1.00	35.09
4557	N	PHE	B	18	18.002	9.572	-14.969	1.00	34.42
4559	CA	PHE	B	18	18.233	10.472	-13.845	1.00	33.65
4561	CB	PHE	B	18	18.831	11.812	-14.264	1.00	33.54
4564	CG	PHE	B	18	19.286	12.629	-13.097	1.00	32.06
4565	CD1	PHE	B	18	20.342	12.202	-12.312	1.00	31.59
4567	CE1	PHE	B	18	20.747	12.940	-11.217	1.00	31.53
4569	CZ	PHE	B	18	20.080	14.100	-10.888	1.00	30.24
4571	CE2	PHE	B	18	19.029	14.516	-11.638	1.00	31.16

FIGURE 3 ~~(Cont.)~~BS

A	B	C	D	E	F	G	H	I	J
4573	CD2	PHE	B	18	18.621	13.779	-12.739	1.00	32.52
4575	C	PHE	B	18	17.015	10.695	-12.946	1.00	33.05
4576	O	PHE	B	18	17.179	10.672	-11.738	1.00	32.55
4577	N	PRO	B	19	15.817	10.901	-13.503	1.00	32.85
4578	CA	PRO	B	19	14.606	11.056	-12.680	1.00	32.66
4580	CB	PRO	B	19	13.497	11.261	-13.722	1.00	32.79
4583	CG	PRO	B	19	14.213	11.795	-14.914	1.00	33.05
4586	CD	PRO	B	19	15.508	11.051	-14.936	1.00	32.96
4589	C	PRO	B	19	14.285	9.869	-11.768	1.00	32.36
4590	O	PRO	B	19	13.759	10.093	-10.685	1.00	31.80
4591	N	GLN	B	20	14.594	8.643	-12.190	1.00	31.98
4593	CA	GLN	B	20	14.399	7.478	-11.329	1.00	32.12
4595	CB	GLN	B	20	14.282	6.175	-12.145	1.00	32.62
4598	CG	GLN	B	20	12.872	5.922	-12.758	1.00	35.79
4601	CD	GLN	B	20	11.784	5.507	-11.736	1.00	38.90
4602	OE1	GLN	B	20	11.382	4.327	-11.677	1.00	40.51
4603	NE2	GLN	B	20	11.292	6.479	-10.956	1.00	40.37
4606	C	GLN	B	20	15.524	7.368	-10.279	1.00	30.90
4607	O	GLN	B	20	15.304	6.829	-9.213	1.00	30.46
4608	N	GLN	B	21	16.715	7.872	-10.583	1.00	30.18
4610	CA	GLN	B	21	17.778	7.963	-9.575	1.00	30.30
4612	CB	GLN	B	21	19.108	8.421	-10.180	1.00	30.56
4615	CG	GLN	B	21	19.929	7.310	-10.799	1.00	33.30
4618	CD	GLN	B	21	20.971	6.745	-9.843	1.00	36.37
4619	OE1	GLN	B	21	21.903	7.457	-9.441	1.00	39.14
4620	NE2	GLN	B	21	20.822	5.474	-9.479	1.00	36.91
4623	C	GLN	B	21	17.364	8.924	-8.464	1.00	29.14
4624	O	GLN	B	21	17.509	8.604	-7.285	1.00	29.47
4625	N	LEU	B	22	16.838	10.086	-8.841	1.00	27.84
4627	CA	LEU	B	22	16.384	11.074	-7.864	1.00	27.57
4629	CB	LEU	B	22	15.793	12.309	-8.546	1.00	27.88
4632	CG	LEU	B	22	16.740	13.324	-9.180	1.00	28.18
4634	CD1	LEU	B	22	15.884	14.370	-9.884	1.00	28.62
4638	CD2	LEU	B	22	17.667	13.973	-8.145	1.00	28.38
4642	C	LEU	B	22	15.317	10.478	-6.961	1.00	27.38
4643	O	LEU	B	22	15.364	10.643	-5.741	1.00	26.09
4644	N	GLU	B	23	14.358	9.786	-7.573	1.00	27.02
4646	CA	GLU	B	23	13.207	9.269	-6.847	1.00	27.65
4648	CB	GLU	B	23	12.098	8.855	-7.825	1.00	28.49
4651	CG	GLU	B	23	11.022	7.981	-7.212	1.00	32.02
4654	CD	GLU	B	23	9.646	8.256	-7.782	1.00	37.15
4655	OE1	GLU	B	23	9.109	9.364	-7.545	1.00	42.58
4656	OE2	GLU	B	23	9.100	7.363	-8.463	1.00	41.15
4657	C	GLU	B	23	13.618	8.112	-5.938	1.00	26.50
4658	O	GLU	B	23	13.115	8.008	-4.823	1.00	26.62
4659	N	ALA	B	24	14.513	7.250	-6.421	1.00	25.43
4661	CA	ALA	B	24	15.092	6.179	-5.610	1.00	24.85
4663	CB	ALA	B	24	16.021	5.297	-6.443	1.00	24.98
4667	C	ALA	B	24	15.864	6.765	-4.421	1.00	24.65
4668	O	ALA	B	24	15.827	6.211	-3.318	1.00	23.25
4669	N	CYS	B	25	16.556	7.885	-4.650	1.00	24.00
4671	CA	CYS	B	25	17.315	8.544	-3.589	1.00	23.64

FIGURE 3 (Cont.)BT

A	B	C	D	E	F	G	H	I	J
4673	CB	CYS	B	25	18.217	9.650	-4.152	1.00	23.72
4676	SG	CYS	B	25	19.117	10.582	-2.885	1.00	22.22
4677	C	CYS	B	25	16.374	9.096	-2.524	1.00	23.27
4678	O	CYS	B	25	16.578	8.876	-1.336	1.00	23.22
4679	N	VAL	B	26	15.323	9.779	-2.945	1.00	23.25
4681	CA	VAL	B	26	14.334	10.280	-2.006	1.00	23.43
4683	CB	VAL	B	26	13.175	10.997	-2.725	1.00	23.51
4685	CG1	VAL	B	26	12.005	11.220	-1.804	1.00	24.68
4689	CG2	VAL	B	26	13.650	12.324	-3.276	1.00	23.07
4693	C	VAL	B	26	13.811	9.132	-1.138	1.00	23.73
4694	O	VAL	B	26	13.641	9.300	0.067	1.00	23.38
4695	N	LYS	B	27	13.581	7.964	-1.737	1.00	23.54
4697	CA	LYS	B	27	13.012	6.852	-0.972	1.00	24.03
4699	CB	LYS	B	27	12.440	5.765	-1.891	1.00	24.27
4702	CG	LYS	B	27	10.995	6.086	-2.256	1.00	27.21
4705	CD	LYS	B	27	10.544	5.567	-3.606	1.00	31.82
4708	CE	LYS	B	27	9.032	5.811	-3.762	1.00	33.94
4711	NZ	LYS	B	27	8.488	5.279	-5.045	1.00	37.62
4715	C	LYS	B	27	14.026	6.287	-0.004	1.00	22.89
4716	O	LYS	B	27	13.699	6.017	1.145	1.00	23.39
4717	N	GLN	B	28	15.257	6.124	-0.468	1.00	22.27
4719	CA	GLN	B	28	16.335	5.645	0.380	1.00	21.89
4721	CB	GLN	B	28	17.623	5.496	-0.423	1.00	21.61
4724	CG	GLN	B	28	18.810	4.946	0.352	1.00	21.80
4727	CD	GLN	B	28	18.683	3.471	0.705	1.00	23.69
4728	OE1	GLN	B	28	19.316	2.999	1.657	1.00	25.82
4729	NE2	GLN	B	28	17.882	2.742	-0.054	1.00	22.57
4732	C	GLN	B	28	16.518	6.604	1.561	1.00	21.61
4733	O	GLN	B	28	16.596	6.163	2.704	1.00	21.00
4734	N	ALA	B	29	16.556	7.906	1.285	1.00	21.58
4736	CA	ALA	B	29	16.835	8.916	2.323	1.00	21.82
4738	CB	ALA	B	29	17.120	10.295	1.691	1.00	21.91
4742	C	ALA	B	29	15.684	9.025	3.317	1.00	21.73
4743	O	ALA	B	29	15.897	9.174	4.508	1.00	21.94
4744	N	ASN	B	30	14.461	8.963	2.822	1.00	22.10
4746	CA	ASN	B	30	13.289	8.996	3.699	1.00	22.38
4748	CB	ASN	B	30	12.013	9.035	2.869	1.00	22.05
4751	CG	ASN	B	30	11.720	10.416	2.319	1.00	23.08
4752	OD1	ASN	B	30	12.374	11.387	2.689	1.00	22.74
4753	ND2	ASN	B	30	10.732	10.510	1.424	1.00	22.09
4756	C	ASN	B	30	13.237	7.812	4.655	1.00	22.64
4757	O	ASN	B	30	12.857	7.962	5.811	1.00	22.97
4758	N	GLN	B	31	13.604	6.637	4.160	1.00	22.84
4760	CA	GLN	B	31	13.624	5.438	4.978	1.00	23.34
4762	CB	GLN	B	31	13.859	4.210	4.085	1.00	23.43
4765	CG	GLN	B	31	14.118	2.893	4.795	1.00	26.33
4768	CD	GLN	B	31	14.528	1.795	3.815	1.00	28.80
4769	OE1	GLN	B	31	15.700	1.679	3.443	1.00	33.07
4770	NE2	GLN	B	31	13.560	1.007	3.378	1.00	32.12
4773	C	GLN	B	31	14.720	5.582	6.039	1.00	23.12
4774	O	GLN	B	31	14.542	5.183	7.178	1.00	23.43
4775	N	ALA	B	32	15.855	6.146	5.653	1.00	22.32

FIGURE 3 (Cont.)BU

A	B	C	D	E	F	G	H	I	J
4777	CA	ALA	B	32	16.974	6.318	6.569	1.00	22.90
4779	CB	ALA	B	32	18.199	6.814	5.818	1.00	22.55
4783	C	ALA	B	32	16.590	7.296	7.679	1.00	22.66
4784	O	ALA	B	32	16.750	6.992	8.861	1.00	22.59
4785	N	LEU	B	33	16.069	8.457	7.288	1.00	22.88
4787	CA	LEU	B	33	15.603	9.462	8.244	1.00	23.19
4789	CB	LEU	B	33	14.980	10.661	7.521	1.00	23.23
4792	CG	LEU	B	33	15.948	11.654	6.869	1.00	24.18
4794	CD1	LEU	B	33	15.253	12.531	5.850	1.00	25.04
4798	CD2	LEU	B	33	16.610	12.528	7.925	1.00	25.95
4802	C	LEU	B	33	14.565	8.869	9.206	1.00	23.67
4803	O	LEU	B	33	14.665	9.037	10.415	1.00	22.94
4804	N	SER	B	34	13.573	8.180	8.654	1.00	24.43
4806	CA	SER	B	34	12.506	7.580	9.458	1.00	25.35
4808	CB	SER	B	34	11.490	6.887	8.551	1.00	25.51
4811	OG	SER	B	34	10.877	7.830	7.706	1.00	26.80
4813	C	SER	B	34	13.043	6.579	10.487	1.00	25.98
4814	O	SER	B	34	12.547	6.525	11.610	1.00	26.04
4815	N	ARG	B	35	14.062	5.813	10.094	1.00	26.60
4817	CA	ARG	B	35	14.700	4.820	10.962	1.00	27.70
4819	CB	ARG	B	35	15.743	3.993	10.185	1.00	28.27
4822	CG	ARG	B	35	15.205	2.761	9.484	1.00	31.67
4825	CD	ARG	B	35	16.207	1.605	9.357	1.00	34.70
4828	NE	ARG	B	35	17.593	2.056	9.140	1.00	36.06
4830	CZ	ARG	B	35	18.083	2.498	7.984	1.00	33.83
4831	NH1	ARG	B	35	17.320	2.570	6.914	1.00	34.48
4834	NH2	ARG	B	35	19.354	2.876	7.903	1.00	33.58
4837	C	ARG	B	35	15.407	5.464	12.148	1.00	27.46
4838	O	ARG	B	35	15.465	4.877	13.237	1.00	27.43
4839	N	PHE	B	36	15.967	6.655	11.926	1.00	27.31
4841	CA	PHE	B	36	16.692	7.373	12.965	1.00	26.91
4843	CB	PHE	B	36	17.758	8.289	12.356	1.00	26.72
4846	CG	PHE	B	36	18.835	7.547	11.623	1.00	24.89
4847	CD1	PHE	B	36	19.206	7.916	10.343	1.00	22.57
4849	CE1	PHE	B	36	20.201	7.220	9.656	1.00	22.79
4851	CZ	PHE	B	36	20.845	6.150	10.267	1.00	23.00
4853	CE2	PHE	B	36	20.493	5.777	11.546	1.00	24.18
4855	CD2	PHE	B	36	19.488	6.473	12.224	1.00	24.53
4857	C	PHE	B	36	15.763	8.164	13.851	1.00	27.56
4858	O	PHE	B	36	16.136	8.505	14.964	1.00	28.14
4859	N	ILE	B	37	14.563	8.457	13.357	1.00	28.06
4861	CA	ILE	B	37	13.570	9.208	14.113	1.00	29.01
4863	CB	ILE	B	37	12.677	10.054	13.160	1.00	29.24
4865	CG1	ILE	B	37	13.470	11.240	12.608	1.00	28.43
4868	CD1	ILE	B	37	12.767	12.003	11.524	1.00	29.06
4872	CG2	ILE	B	37	11.412	10.552	13.876	1.00	30.14
4876	C	ILE	B	37	12.719	8.257	14.959	1.00	29.75
4877	O	ILE	B	37	12.120	8.678	15.948	1.00	30.10
4878	N	ALA	B	38	12.698	6.977	14.580	1.00	30.36
4880	CA	ALA	B	38	11.784	5.995	15.172	1.00	30.63
4882	CB	ALA	B	38	11.849	4.666	14.409	1.00	30.80
4886	C	ALA	B	38	12.021	5.762	16.651	1.00	30.90

FIGURE 3 ~~(Cont.)~~BV

A	B	C	D	E	F	G	H	I	J
4887	O	ALA	B	38	11.052	5.739	17.415	1.00	31.31
4888	N	PRO	B	39	13.278	5.595	17.074	1.00	31.28
4889	CA	PRO	B	39	13.573	5.370	18.494	1.00	31.54
4891	CB	PRO	B	39	15.045	4.922	18.489	1.00	31.77
4894	CG	PRO	B	39	15.425	4.741	17.062	1.00	32.00
4897	CD	PRO	B	39	14.512	5.594	16.270	1.00	31.28
4900	C	PRO	B	39	13.423	6.610	19.377	1.00	31.62
4901	O	PRO	B	39	13.551	6.466	20.594	1.00	32.39
4902	N	LEU	B	40	13.184	7.790	18.794	1.00	30.70
4904	CA	LEU	B	40	13.053	9.012	19.575	1.00	30.07
4906	CB	LEU	B	40	12.980	10.253	18.670	1.00	30.11
4909	CG	LEU	B	40	14.228	10.593	17.836	1.00	30.37
4911	CD1	LEU	B	40	13.985	11.886	17.056	1.00	30.25
4915	CD2	LEU	B	40	15.502	10.691	18.687	1.00	30.52
4919	C	LEU	B	40	11.801	8.963	20.448	1.00	29.37
4920	O	LEU	B	40	10.747	8.494	20.005	1.00	29.73
4921	N	PRO	B	41	11.903	9.477	21.669	1.00	28.40
4922	CA	PRO	B	41	10.738	9.551	22.553	1.00	28.09
4924	CB	PRO	B	41	11.355	9.872	23.921	1.00	28.24
4927	CG	PRO	B	41	12.658	10.565	23.613	1.00	28.08
4930	CD	PRO	B	41	13.115	10.033	22.301	1.00	28.09
4933	C	PRO	B	41	9.796	10.657	22.100	1.00	27.75
4934	O	PRO	B	41	10.119	11.411	21.154	1.00	26.90
4935	N	PHE	B	42	8.630	10.724	22.739	1.00	27.16
4937	CA	PHE	B	42	7.644	11.774	22.477	1.00	27.19
4939	CB	PHE	B	42	8.224	13.158	22.776	1.00	27.06
4942	CG	PHE	B	42	8.887	13.259	24.118	1.00	27.64
4943	CD1	PHE	B	42	8.136	13.124	25.279	1.00	28.66
4945	CE1	PHE	B	42	8.732	13.207	26.518	1.00	29.45
4947	CZ	PHE	B	42	10.096	13.439	26.617	1.00	28.49
4949	CE2	PHE	B	42	10.863	13.574	25.475	1.00	27.66
4951	CD2	PHE	B	42	10.260	13.485	24.226	1.00	27.57
4953	C	PHE	B	42	7.094	11.730	21.053	1.00	27.15
4954	O	PHE	B	42	6.729	12.755	20.491	1.00	26.43
4955	N	GLN	B	43	7.015	10.534	20.489	1.00	27.91
4957	CA	GLN	B	43	6.310	10.320	19.224	1.00	28.60
4959	CB	GLN	B	43	6.294	8.834	18.858	1.00	28.40
4962	CG	GLN	B	43	7.659	8.201	18.665	1.00	28.70
4965	CD	GLN	B	43	8.379	8.718	17.438	1.00	28.74
4966	OE1	GLN	B	43	7.765	8.927	16.394	1.00	29.53
4967	NE2	GLN	B	43	9.685	8.915	17.558	1.00	28.45
4970	C	GLN	B	43	4.868	10.796	19.363	1.00	29.43
4971	O	GLN	B	43	4.275	10.720	20.449	1.00	30.02
4972	N	ASN	B	44	4.311	11.291	18.268	1.00	30.07
4974	CA	ASN	B	44	2.942	11.787	18.226	1.00	30.82
4976	CB	ASN	B	44	1.943	10.631	18.396	1.00	31.34
4979	CG	ASN	B	44	2.264	9.445	17.492	1.00	32.36
4980	OD1	ASN	B	44	2.338	9.579	16.261	1.00	35.83
4981	ND2	ASN	B	44	2.480	8.288	18.096	1.00	33.67
4984	C	ASN	B	44	2.684	12.898	19.244	1.00	30.94
4985	O	ASN	B	44	1.596	12.983	19.805	1.00	31.98
4986	N	THR	B	45	3.705	13.716	19.507	1.00	30.13

FIGURE 3 (Cont.)BW

A	B	C	D	E	F	G	H	I	J
4988	CA	THR	B	45	3.529	14.982	20.201	1.00	29.44
4990	CB	THR	B	45	4.399	15.055	21.470	1.00	29.55
4992	OG1	THR	B	45	5.790	15.106	21.123	1.00	29.59
4994	CG2	THR	B	45	4.249	13.787	22.313	1.00	30.13
4998	C	THR	B	45	3.901	16.083	19.216	1.00	28.76
4999	O	THR	B	45	4.574	15.800	18.231	1.00	29.08
5000	N	PRO	B	46	3.458	17.318	19.450	1.00	28.09
5001	CA	PRO	B	46	3.684	18.421	18.494	1.00	27.28
5003	CB	PRO	B	46	3.174	19.652	19.252	1.00	27.82
5006	CG	PRO	B	46	2.115	19.111	20.181	1.00	28.40
5009	CD	PRO	B	46	2.640	17.750	20.605	1.00	28.19
5012	C	PRO	B	46	5.135	18.643	18.041	1.00	26.19
5013	O	PRO	B	46	5.357	18.854	16.853	1.00	25.60
5014	N	VAL	B	47	6.100	18.595	18.957	1.00	24.76
5016	CA	VAL	B	47	7.479	18.902	18.602	1.00	23.94
5018	CB	VAL	B	47	8.365	19.173	19.859	1.00	24.25
5020	CG1	VAL	B	47	8.593	17.904	20.684	1.00	24.46
5024	CG2	VAL	B	47	9.678	19.801	19.452	1.00	25.37
5028	C	VAL	B	47	8.074	17.824	17.690	1.00	22.86
5029	O	VAL	B	47	8.719	18.150	16.704	1.00	21.98
5030	N	VAL	B	48	7.822	16.549	17.991	1.00	22.17
5032	CA	VAL	B	48	8.303	15.456	17.145	1.00	22.05
5034	CB	VAL	B	48	8.227	14.101	17.872	1.00	22.22
5036	CG1	VAL	B	48	8.620	12.960	16.951	1.00	22.38
5040	CG2	VAL	B	48	9.132	14.128	19.090	1.00	22.62
5044	C	VAL	B	48	7.547	15.414	15.816	1.00	22.15
5045	O	VAL	B	48	8.108	15.076	14.775	1.00	21.53
5046	N	GLU	B	49	6.273	15.760	15.844	1.00	22.30
5048	CA	GLU	B	49	5.501	15.839	14.612	1.00	23.31
5050	CB	GLU	B	49	4.020	16.062	14.906	1.00	23.97
5053	CG	GLU	B	49	3.349	14.847	15.529	1.00	27.97
5056	CD	GLU	B	49	1.902	15.107	15.899	1.00	32.93
5057	OE1	GLU	B	49	1.410	16.237	15.650	1.00	37.74
5058	OE2	GLU	B	49	1.263	14.182	16.446	1.00	36.88
5059	C	GLU	B	49	6.023	16.965	13.727	1.00	22.40
5060	O	GLU	B	49	6.016	16.837	12.516	1.00	21.26
5061	N	THR	B	50	6.497	18.044	14.344	1.00	21.39
5063	CA	THR	B	50	7.105	19.143	13.607	1.00	21.78
5065	CB	THR	B	50	7.382	20.353	14.534	1.00	22.24
5067	OG1	THR	B	50	6.174	20.767	15.191	1.00	21.33
5069	CG2	THR	B	50	7.803	21.573	13.727	1.00	22.96
5073	C	THR	B	50	8.406	18.684	12.964	1.00	21.83
5074	O	THR	B	50	8.671	19.001	11.808	1.00	21.23
5075	N	MET	B	51	9.220	17.953	13.728	1.00	21.95
5077	CA	MET	B	51	10.470	17.408	13.215	1.00	21.91
5079	CB	MET	B	51	11.207	16.630	14.299	1.00	21.87
5082	CG	MET	B	51	11.735	17.485	15.441	1.00	20.93
5085	SD	MET	B	51	12.315	16.444	16.774	1.00	22.35
5086	CE	MET	B	51	13.754	15.689	16.047	1.00	23.07
5090	C	MET	B	51	10.221	16.502	12.014	1.00	22.56
5091	O	MET	B	51	10.951	16.565	11.024	1.00	22.83
5092	N	GLN	B	52	9.179	15.676	12.088	1.00	23.09

FIGURE 3 (Cont.)BX

A	B	C	D	E	F	G	H	I	J
5094	CA	GLN	B	52	8.895	14.714	11.016	1.00	23.09
5096	CB	GLN	B	52	7.843	13.694	11.460	1.00	23.18
5099	CG	GLN	B	52	8.386	12.700	12.456	1.00	24.11
5102	CD	GLN	B	52	7.334	11.743	12.961	1.00	26.66
5103	OE1	GLN	B	52	7.463	10.525	12.791	1.00	28.62
5104	NE2	GLN	B	52	6.304	12.280	13.601	1.00	23.91
5107	C	GLN	B	52	8.393	15.435	9.787	1.00	22.65
5108	O	GLN	B	52	8.764	15.123	8.661	1.00	22.15
5109	N	TYR	B	53	7.531	16.402	10.028	1.00	22.64
5111	CA	TYR	B	53	6.942	17.213	8.974	1.00	22.81
5113	CB	TYR	B	53	5.939	18.145	9.647	1.00	23.23
5116	CG	TYR	B	53	5.133	19.066	8.784	1.00	24.77
5117	CD1	TYR	B	53	3.855	18.706	8.346	1.00	27.29
5119	CE1	TYR	B	53	3.089	19.572	7.587	1.00	28.69
5121	CZ	TYR	B	53	3.582	20.820	7.286	1.00	28.49
5122	OH	TYR	B	53	2.827	21.673	6.537	1.00	28.74
5124	CE2	TYR	B	53	4.844	21.209	7.727	1.00	27.93
5126	CD2	TYR	B	53	5.600	20.335	8.477	1.00	26.79
5128	C	TYR	B	53	8.051	17.978	8.237	1.00	22.85
5129	O	TYR	B	53	8.114	17.976	7.010	1.00	22.68
5130	N	GLY	B	54	8.948	18.591	9.005	1.00	22.75
5132	CA	GLY	B	54	10.014	19.408	8.455	1.00	22.25
5135	C	GLY	B	54	11.071	18.608	7.738	1.00	22.08
5136	O	GLY	B	54	11.669	19.088	6.782	1.00	21.36
5137	N	ALA	B	55	11.310	17.384	8.201	1.00	22.33
5139	CA	ALA	B	55	12.382	16.568	7.656	1.00	22.52
5141	CB	ALA	B	55	12.996	15.714	8.733	1.00	22.31
5145	C	ALA	B	55	11.925	15.698	6.492	1.00	23.07
5146	O	ALA	B	55	12.692	15.487	5.548	1.00	22.77
5147	N	LEU	B	56	10.682	15.220	6.538	1.00	23.33
5149	CA	LEU	B	56	10.265	14.079	5.705	1.00	24.30
5151	CB	LEU	B	56	9.706	12.960	6.586	1.00	24.12
5154	CG	LEU	B	56	10.789	12.220	7.367	1.00	24.95
5156	CD1	LEU	B	56	10.177	11.362	8.448	1.00	25.81
5160	CD2	LEU	B	56	11.624	11.386	6.415	1.00	25.72
5164	C	LEU	B	56	9.241	14.390	4.610	1.00	24.83
5165	O	LEU	B	56	9.168	13.668	3.615	1.00	24.82
5166	N	LEU	B	57	8.480	15.459	4.784	1.00	25.44
5168	CA	LEU	B	57	7.363	15.761	3.890	1.00	26.38
5170	CB	LEU	B	57	6.196	16.353	4.683	1.00	26.51
5173	CG	LEU	B	57	4.851	15.625	4.607	1.00	29.53
5175	CD1	LEU	B	57	4.953	14.108	4.807	1.00	30.58
5179	CD2	LEU	B	57	3.880	16.228	5.625	1.00	30.77
5183	C	LEU	B	57	7.833	16.671	2.741	1.00	26.06
5184	O	LEU	B	57	7.862	17.895	2.846	1.00	27.01
5185	N	GLY	B	58	8.237	16.048	1.651	1.00	25.60
5187	CA	GLY	B	58	8.677	16.778	0.477	1.00	25.47
5190	C	GLY	B	58	10.152	17.095	0.529	1.00	24.67
5191	O	GLY	B	58	10.821	16.878	1.542	1.00	24.85
5192	N	GLY	B	59	10.655	17.628	-0.575	1.00	24.17
5194	CA	GLY	B	59	12.046	18.001	-0.702	1.00	23.50
5197	C	GLY	B	59	12.688	17.037	-1.671	1.00	23.34

FIGURE 3 ~~(Cont.)~~BY

A	B	C	D	E	F	G	H	I	J
5198	O	GLY	B	59	12.221	15.901	-1.822	1.00	23.79
5199	N	LYS	B	60	13.776	17.465	-2.305	1.00	22.25
5201	CA	LYS	B	60	14.378	16.698	-3.397	1.00	21.47
5203	CB	LYS	B	60	14.964	17.634	-4.446	1.00	21.33
5206	CG	LYS	B	60	13.989	18.633	-5.009	1.00	21.64
5209	CD	LYS	B	60	14.690	19.563	-5.983	1.00	20.05
5212	CE	LYS	B	60	15.503	20.635	-5.285	1.00	20.61
5215	NZ	LYS	B	60	14.661	21.571	-4.488	1.00	18.47
5219	C	LYS	B	60	15.473	15.764	-2.916	1.00	20.81
5220	O	LYS	B	60	15.930	14.904	-3.680	1.00	19.71
5221	N	ARG	B	61	15.873	15.934	-1.651	1.00	19.67
5223	CA	ARG	B	61	16.956	15.168	-1.037	1.00	19.66
5225	CB	ARG	B	61	16.531	13.713	-0.785	1.00	19.62
5228	CG	ARG	B	61	15.280	13.581	0.031	1.00	20.32
5231	CD	ARG	B	61	15.456	13.814	1.534	1.00	21.36
5234	NE	ARG	B	61	14.145	13.667	2.159	1.00	22.35
5236	CZ	ARG	B	61	13.232	14.625	2.243	1.00	24.57
5237	NH1	ARG	B	61	13.491	15.867	1.836	1.00	25.55
5240	NH2	ARG	B	61	12.042	14.347	2.754	1.00	25.42
5243	C	ARG	B	61	18.218	15.188	-1.878	1.00	19.19
5244	O	ARG	B	61	18.871	14.162	-2.042	1.00	19.59
5245	N	LEU	B	62	18.575	16.345	-2.419	1.00	18.57
5247	CA	LEU	B	62	19.781	16.421	-3.233	1.00	18.09
5249	CB	LEU	B	62	19.801	17.700	-4.043	1.00	18.16
5252	CG	LEU	B	62	18.659	17.854	-5.069	1.00	17.75
5254	CD1	LEU	B	62	18.918	19.010	-5.960	1.00	17.68
5258	CD2	LEU	B	62	18.460	16.582	-5.902	1.00	17.92
5262	C	LEU	B	62	21.050	16.265	-2.398	1.00	18.27
5263	O	LEU	B	62	22.075	15.828	-2.904	1.00	19.36
5264	N	ARG	B	63	20.984	16.589	-1.118	1.00	18.60
5266	CA	ARG	B	63	22.152	16.472	-0.263	1.00	18.77
5268	CB	ARG	B	63	22.052	17.389	0.948	1.00	18.34
5271	CG	ARG	B	63	22.255	18.855	0.557	1.00	18.92
5274	CD	ARG	B	63	21.763	19.861	1.576	1.00	19.63
5277	NE	ARG	B	63	21.626	21.189	0.993	1.00	18.86
5279	CZ	ARG	B	63	20.623	21.574	0.213	1.00	20.23
5280	NH1	ARG	B	63	20.591	22.816	-0.258	1.00	20.75
5283	NH2	ARG	B	63	19.642	20.736	-0.106	1.00	20.23
5286	C	ARG	B	63	22.421	14.999	0.076	1.00	19.10
5287	O	ARG	B	63	23.547	14.561	-0.077	1.00	19.88
5288	N	PRO	B	64	21.423	14.225	0.504	1.00	19.43
5289	CA	PRO	B	64	21.571	12.764	0.495	1.00	19.41
5291	CB	PRO	B	64	20.168	12.271	0.822	1.00	20.11
5294	CG	PRO	B	64	19.619	13.337	1.712	1.00	19.65
5297	CD	PRO	B	64	20.136	14.628	1.091	1.00	19.55
5300	C	PRO	B	64	22.061	12.230	-0.851	1.00	18.78
5301	O	PRO	B	64	22.971	11.411	-0.850	1.00	19.31
5302	N	PHE	B	65	21.512	12.708	-1.965	1.00	18.78
5304	CA	PHE	B	65	21.994	12.301	-3.290	1.00	18.13
5306	CB	PHE	B	65	21.301	13.089	-4.406	1.00	18.17
5309	CG	PHE	B	65	21.440	12.462	-5.768	1.00	19.67
5310	CD1	PHE	B	65	22.618	12.595	-6.496	1.00	21.70

FIGURE 3 ~~(Cont.)~~BZ

A	B	C	D	E	F	G	H	I	J
5312	CE1	PHE	B	65	22.745	12.007	-7.755	1.00	22.62
5314	CZ	PHE	B	65	21.697	11.280	-8.296	1.00	23.33
5316	CE2	PHE	B	65	20.532	11.138	-7.587	1.00	23.93
5318	CD2	PHE	B	65	20.400	11.730	-6.324	1.00	22.20
5320	C	PHE	B	65	23.518	12.444	-3.401	1.00	18.01
5321	O	PHE	B	65	24.194	11.528	-3.851	1.00	17.71
5322	N	LEU	B	66	24.042	13.591	-2.986	1.00	17.36
5324	CA	LEU	B	66	25.470	13.851	-3.011	1.00	17.79
5326	CB	LEU	B	66	25.775	15.297	-2.615	1.00	17.54
5329	CG	LEU	B	66	25.431	16.355	-3.650	1.00	18.09
5331	CD1	LEU	B	66	25.477	17.733	-3.004	1.00	20.27
5335	CD2	LEU	B	66	26.378	16.312	-4.830	1.00	18.85
5339	C	LEU	B	66	26.245	12.913	-2.104	1.00	17.24
5340	O	LEU	B	66	27.325	12.470	-2.464	1.00	17.66
5341	N	VAL	B	67	25.717	12.633	-0.920	1.00	16.80
5343	CA	VAL	B	67	26.388	11.711	-0.011	1.00	16.74
5345	CB	VAL	B	67	25.658	11.640	1.340	1.00	16.98
5347	CG1	VAL	B	67	26.180	10.504	2.196	1.00	16.26
5351	CG2	VAL	B	67	25.754	13.004	2.088	1.00	17.68
5355	C	VAL	B	67	26.465	10.322	-0.656	1.00	16.74
5356	O	VAL	B	67	27.536	9.725	-0.718	1.00	15.63
5357	N	TYR	B	68	25.315	9.830	-1.120	1.00	17.27
5359	CA	TYR	B	68	25.226	8.520	-1.767	1.00	18.14
5361	CB	TYR	B	68	23.790	8.181	-2.162	1.00	18.15
5364	CG	TYR	B	68	22.884	7.903	-1.001	1.00	17.89
5365	CD1	TYR	B	68	23.205	6.940	-0.059	1.00	19.51
5367	CE1	TYR	B	68	22.357	6.678	1.022	1.00	18.10
5369	CZ	TYR	B	68	21.198	7.396	1.155	1.00	18.28
5370	OH	TYR	B	68	20.351	7.135	2.215	1.00	19.90
5372	CE2	TYR	B	68	20.866	8.363	0.221	1.00	18.45
5374	CD2	TYR	B	68	21.699	8.599	-0.846	1.00	18.98
5376	C	TYR	B	68	26.082	8.438	-3.015	1.00	17.83
5377	O	TYR	B	68	26.788	7.478	-3.201	1.00	17.93
5378	N	ALA	B	69	26.031	9.456	-3.868	1.00	18.14
5380	CA	ALA	B	69	26.687	9.377	-5.168	1.00	17.87
5382	CB	ALA	B	69	26.264	10.525	-6.039	1.00	18.36
5386	C	ALA	B	69	28.200	9.387	-4.975	1.00	18.40
5387	O	ALA	B	69	28.960	8.703	-5.696	1.00	18.10
5388	N	THR	B	70	28.639	10.155	-3.985	1.00	18.02
5390	CA	THR	B	70	30.055	10.258	-3.691	1.00	18.66
5392	CB	THR	B	70	30.300	11.424	-2.750	1.00	17.72
5394	OG1	THR	B	70	29.858	12.636	-3.373	1.00	18.73
5396	CG2	THR	B	70	31.801	11.638	-2.534	1.00	19.07
5400	C	THR	B	70	30.634	8.968	-3.097	1.00	19.24
5401	O	THR	B	70	31.644	8.449	-3.592	1.00	19.75
5402	N	GLY	B	71	29.999	8.474	-2.036	1.00	19.50
5404	CA	GLY	B	71	30.432	7.259	-1.389	1.00	20.08
5407	C	GLY	B	71	30.417	6.071	-2.343	1.00	20.27
5408	O	GLY	B	71	31.314	5.231	-2.310	1.00	20.87
5409	N	HIS	B	72	29.379	6.008	-3.169	1.00	20.75
5411	CA	HIS	B	72	29.201	4.952	-4.163	1.00	21.28
5413	CB	HIS	B	72	27.909	5.167	-4.955	1.00	20.79

FIGURE 3 (Cont.)CA

A	B	C	D	E	F	G	H	I	J
5416	CG	HIS	B	72	26.666	4.749	-4.233	1.00	20.15
5417	ND1	HIS	B	72	25.407	4.975	-4.744	1.00	18.98
5419	CE1	HIS	B	72	24.500	4.502	-3.911	1.00	20.13
5421	NE2	HIS	B	72	25.126	3.949	-2.887	1.00	20.74
5423	CD2	HIS	B	72	26.482	4.101	-3.059	1.00	21.64
5425	C	HIS	B	72	30.361	4.878	-5.151	1.00	21.89
5426	O	HIS	B	72	30.692	3.791	-5.606	1.00	21.76
5427	N	MET	B	73	30.960	6.023	-5.493	1.00	22.15
5429	CA	MET	B	73	32.157	6.051	-6.357	1.00	23.42
5431	CB	MET	B	73	32.672	7.481	-6.565	1.00	23.57
5434	CG	MET	B	73	31.804	8.325	-7.471	1.00	24.99
5437	SD	MET	B	73	32.611	9.844	-8.067	1.00	26.07
5438	CE	MET	B	73	33.270	10.463	-6.588	1.00	25.93
5442	C	MET	B	73	33.303	5.200	-5.819	1.00	23.68
5443	O	MET	B	73	34.094	4.657	-6.595	1.00	24.77
5444	N	PHE	B	74	33.405	5.105	-4.502	1.00	23.69
5446	CA	PHE	B	74	34.474	4.342	-3.856	1.00	23.70
5448	CB	PHE	B	74	35.073	5.171	-2.720	1.00	23.12
5451	CG	PHE	B	74	35.419	6.571	-3.134	1.00	23.22
5452	CD1	PHE	B	74	34.539	7.620	-2.887	1.00	22.52
5454	CE1	PHE	B	74	34.842	8.909	-3.297	1.00	21.95
5456	CZ	PHE	B	74	36.029	9.160	-3.967	1.00	23.61
5458	CE2	PHE	B	74	36.910	8.116	-4.230	1.00	22.42
5460	CD2	PHE	B	74	36.604	6.834	-3.818	1.00	23.20
5462	C	PHE	B	74	34.016	2.986	-3.339	1.00	23.73
5463	O	PHE	B	74	34.751	2.309	-2.625	1.00	23.67
5464	N	GLY	B	75	32.791	2.607	-3.686	1.00	23.96
5466	CA	GLY	B	75	32.273	1.287	-3.397	1.00	24.04
5469	C	GLY	B	75	31.674	1.153	-2.023	1.00	23.99
5470	O	GLY	B	75	31.462	0.038	-1.543	1.00	23.68
5471	N	VAL	B	76	31.385	2.278	-1.375	1.00	23.71
5473	CA	VAL	B	76	30.866	2.207	-0.020	1.00	23.08
5475	CB	BVAL	B	76	31.048	3.547	0.736	0.35	22.92
5476	CB	AVAL	B	76	31.192	3.459	0.840	0.65	23.42
5479	CG1	BVAL	B	76	30.368	3.508	2.114	0.35	22.09
5480	CG1	AVAL	B	76	32.625	3.934	0.590	0.65	23.81
5487	CG2	BVAL	B	76	32.527	3.883	0.872	0.35	23.15
5488	CG2	AVAL	B	76	30.219	4.544	0.625	0.65	24.67
5495	C	VAL	B	76	29.387	1.847	-0.088	1.00	22.55
5496	O	VAL	B	76	28.660	2.300	-0.965	1.00	21.42
5497	N	SER	B	77	28.987	0.968	0.819	1.00	22.22
5499	CA	SER	B	77	27.645	0.429	0.868	1.00	22.25
5501	CB	SER	B	77	27.539	-0.621	1.979	1.00	22.22
5504	OG	SER	B	77	26.202	-1.078	2.137	1.00	22.42
5506	C	SER	B	77	26.656	1.550	1.108	1.00	22.33
5507	O	SER	B	77	26.919	2.462	1.898	1.00	21.77
5508	N	THR	B	78	25.534	1.480	0.394	1.00	21.99
5510	CA	THR	B	78	24.431	2.400	0.559	1.00	22.06
5512	CB	THR	B	78	23.259	1.990	-0.367	1.00	22.16
5514	OG1	THR	B	78	23.685	2.032	-1.732	1.00	23.21
5516	CG2	THR	B	78	22.126	2.999	-0.303	1.00	22.58
5520	C	THR	B	78	23.949	2.433	1.997	1.00	21.59

FIGURE 3 (Cont.)CB

A	B	C	D	E	F	G	H	I	J
5521	O	THR	B	78	23.618	3.500	2.527	1.00	21.04
5522	N	ASN	B	79	23.897	1.261	2.628	1.00	21.29
5524	CA	ASN	B	79	23.467	1.170	4.022	1.00	21.08
5526	CB	ASN	B	79	23.358	-0.293	4.454	1.00	21.68
5529	CG	ASN	B	79	23.046	-0.442	5.923	1.00	21.92
5530	OD1	ASN	B	79	21.903	-0.297	6.343	1.00	23.33
5531	ND2	ASN	B	79	24.060	-0.747	6.706	1.00	22.60
5534	C	ASN	B	79	24.404	1.930	4.963	1.00	20.60
5535	O	ASN	B	79	23.950	2.532	5.920	1.00	19.95
5536	N	THR	B	80	25.708	1.876	4.708	1.00	20.20
5538	CA	THR	B	80	26.661	2.698	5.453	1.00	20.29
5540	CB	THR	B	80	28.086	2.339	5.017	1.00	20.31
5542	OG1	THR	B	80	28.386	1.014	5.482	1.00	20.98
5544	CG2	THR	B	80	29.139	3.242	5.699	1.00	21.55
5548	C	THR	B	80	26.390	4.199	5.257	1.00	20.17
5549	O	THR	B	80	26.440	4.994	6.218	1.00	20.64
5550	N	LEU	B	81	26.078	4.560	4.013	1.00	19.46
5552	CA	LEU	B	81	25.883	5.947	3.604	1.00	19.22
5554	CB	LEU	B	81	25.952	6.044	2.077	1.00	18.97
5557	CG	LEU	B	81	27.376	5.905	1.533	1.00	19.26
5559	CD1	LEU	B	81	27.370	5.638	0.037	1.00	20.15
5563	CD2	LEU	B	81	28.251	7.121	1.875	1.00	20.46
5567	C	LEU	B	81	24.584	6.574	4.113	1.00	19.19
5568	O	LEU	B	81	24.445	7.794	4.139	1.00	18.91
5569	N	ASP	B	82	23.641	5.746	4.523	1.00	19.51
5571	CA	ASP	B	82	22.393	6.219	5.106	1.00	19.28
5573	CB	ASP	B	82	21.559	5.046	5.616	1.00	19.89
5576	CG	ASP	B	82	20.654	4.406	4.552	1.00	21.00
5577	OD1	ASP	B	82	20.591	4.823	3.365	1.00	21.03
5578	OD2	ASP	B	82	19.938	3.431	4.867	1.00	24.24
5579	C	ASP	B	82	22.645	7.167	6.297	1.00	18.72
5580	O	ASP	B	82	21.924	8.147	6.462	1.00	18.18
5581	N	ALA	B	83	23.639	6.861	7.130	1.00	18.70
5583	CA	ALA	B	83	23.955	7.700	8.290	1.00	19.48
5585	CB	ALA	B	83	25.006	7.061	9.204	1.00	19.64
5589	C	ALA	B	83	24.360	9.113	7.894	1.00	19.16
5590	O	ALA	B	83	23.679	10.049	8.257	1.00	18.92
5591	N	PRO	B	84	25.451	9.305	7.163	1.00	19.56
5592	CA	PRO	B	84	25.781	10.672	6.739	1.00	19.16
5594	CB	PRO	B	84	27.114	10.519	6.004	1.00	19.21
5597	CG	PRO	B	84	27.166	9.070	5.606	1.00	19.67
5600	CD	PRO	B	84	26.446	8.323	6.694	1.00	19.64
5603	C	PRO	B	84	24.692	11.299	5.856	1.00	18.58
5604	O	PRO	B	84	24.509	12.510	5.924	1.00	18.13
5605	N	ALA	B	85	23.975	10.506	5.063	1.00	18.37
5607	CA	ALA	B	85	22.891	11.038	4.225	1.00	18.51
5609	CB	ALA	B	85	22.314	9.952	3.312	1.00	18.83
5613	C	ALA	B	85	21.790	11.644	5.073	1.00	18.64
5614	O	ALA	B	85	21.313	12.749	4.811	1.00	19.06
5615	N	ALA	B	86	21.407	10.928	6.114	1.00	18.40
5617	CA	ALA	B	86	20.360	11.383	7.010	1.00	18.11
5619	CB	ALA	B	86	19.906	10.245	7.903	1.00	18.05

FIGURE 3 ~~(Cont.)~~<u>CC</u>

A	B	C	D	E	F	G	H	I	J
5623	C	ALA	B	86	20.855	12.566	7.841	1.00	17.48
5624	O	ALA	B	86	20.123	13.505	8.071	1.00	16.95
5625	N	ALA	B	87	22.105	12.525	8.281	1.00	17.41
5627	CA	ALA	B	87	22.630	13.600	9.115	1.00	17.40
5629	CB	ALA	B	87	23.982	13.244	9.638	1.00	17.13
5633	C	ALA	B	87	22.680	14.917	8.335	1.00	17.61
5634	O	ALA	B	87	22.298	15.947	8.858	1.00	17.33
5635	N	VAL	B	88	23.143	14.893	7.091	1.00	18.42
5637	CA	VAL	B	88	23.208	16.146	6.304	1.00	18.96
5639	CB	BVAL	B	88	24.038	16.002	4.993	0.35	18.97
5640	CB	AVAL	B	88	23.983	16.016	4.957	0.65	19.14
5643	CG1	BVAL	B	88	23.256	15.295	3.906	0.35	19.73
5644	CG1	AVAL	B	88	25.429	15.726	5.214	0.65	19.11
5651	CG2	BVAL	B	88	24.517	17.378	4.509	0.35	18.57
5652	CG2	AVAL	B	88	23.381	14.977	4.031	0.65	20.34
5659	C	VAL	B	88	21.813	16.685	6.031	1.00	19.05
5660	O	VAL	B	88	21.610	17.902	6.048	1.00	19.83
5661	N	GLU	B	89	20.858	15.786	5.828	1.00	18.96
5663	CA	GLU	B	89	19.479	16.181	5.611	1.00	19.29
5665	CB	GLU	B	89	18.657	15.024	5.045	1.00	19.83
5668	CG	GLU	B	89	17.271	15.429	4.550	1.00	20.18
5671	CD	GLU	B	89	17.276	16.380	3.353	1.00	21.04
5672	OE1	GLU	B	89	16.175	16.831	2.956	1.00	20.80
5673	OE2	GLU	B	89	18.352	16.669	2.784	1.00	22.55
5674	C	GLU	B	89	18.816	16.727	6.868	1.00	19.09
5675	O	GLU	B	89	17.964	17.587	6.761	1.00	18.76
5676	N	CYS	B	90	19.205	16.246	8.053	1.00	19.19
5678	CA	CYS	B	90	18.694	16.808	9.313	1.00	18.68
5680	CB	CYS	B	90	19.186	16.019	10.519	1.00	19.12
5683	SG	CYS	B	90	18.326	14.474	10.771	1.00	22.59
5684	C	CYS	B	90	19.160	18.255	9.485	1.00	17.90
5685	O	CYS	B	90	18.407	19.095	9.978	1.00	17.58
5686	N	ILE	B	91	20.416	18.524	9.129	1.00	16.55
5688	CA	ILE	B	91	20.951	19.877	9.214	1.00	16.20
5690	CB	ILE	B	91	22.468	19.934	8.896	1.00	15.98
5692	CG1	ILE	B	91	23.261	19.204	9.970	1.00	15.40
5695	CD1	ILE	B	91	23.203	19.886	11.342	1.00	17.23
5699	CG2	ILE	B	91	22.941	21.391	8.777	1.00	15.29
5703	C	ILE	B	91	20.200	20.722	8.215	1.00	15.87
5704	O	ILE	B	91	19.770	21.815	8.533	1.00	15.70
5705	N	HIS	B	92	20.067	20.215	6.992	1.00	15.91
5707	CA	HIS	B	92	19.330	20.914	5.957	1.00	16.10
5709	CB	HIS	B	92	19.247	20.072	4.687	1.00	16.66
5712	CG	HIS	B	92	18.572	20.782	3.567	1.00	15.86
5713	ND1	HIS	B	92	17.518	20.240	2.860	1.00	19.53
5715	CE1	HIS	B	92	17.127	21.104	1.941	1.00	17.62
5717	NE2	HIS	B	92	17.871	22.190	2.043	1.00	19.93
5719	CD2	HIS	B	92	18.776	22.017	3.057	1.00	15.34
5721	C	HIS	B	92	17.923	21.259	6.424	1.00	17.04
5722	O	HIS	B	92	17.524	22.425	6.412	1.00	16.67
5723	N	ALA	B	93	17.193	20.243	6.885	1.00	17.19
5725	CA	ALA	B	93	15.809	20.414	7.334	1.00	17.14

FIGURE 3 (Cont.)CD

A	B	C	D	E	F	G	H	I	J
5727	CB	ALA	B	93	15.236	19.074	7.793	1.00	17.69
5731	C	ALA	B	93	15.681	21.456	8.452	1.00	17.97
5732	O	ALA	B	93	14.806	22.325	8.400	1.00	17.24
5733	N	TYR	B	94	16.570	21.389	9.449	1.00	17.80
5735	CA	TYR	B	94	16.550	22.348	10.560	1.00	17.32
5737	CB	TYR	B	94	17.580	21.968	11.647	1.00	18.17
5740	CG	TYR	B	94	18.635	23.015	11.933	1.00	19.38
5741	CD1	TYR	B	94	18.308	24.219	12.556	1.00	22.96
5743	CE1	TYR	B	94	19.290	25.186	12.809	1.00	23.47
5745	CZ	TYR	B	94	20.601	24.932	12.424	1.00	23.58
5746	OH	TYR	B	94	21.596	25.839	12.653	1.00	22.83
5748	CE2	TYR	B	94	20.935	23.736	11.815	1.00	21.94
5750	CD2	TYR	B	94	19.963	22.802	11.571	1.00	20.83
5752	C	TYR	B	94	16.810	23.765	10.042	1.00	16.90
5753	O	TYR	B	94	16.187	24.727	10.489	1.00	16.75
5754	N	SER	B	95	17.730	23.891	9.098	1.00	16.44
5756	CA	SER	B	95	18.097	25.192	8.581	1.00	17.14
5758	CB	SER	B	95	19.263	25.083	7.593	1.00	16.73
5761	OG	SER	B	95	18.840	24.597	6.337	1.00	18.73
5763	C	SER	B	95	16.887	25.851	7.924	1.00	17.47
5764	O	SER	B	95	16.686	27.050	8.047	1.00	17.44
5765	N	LEU	B	96	16.089	25.064	7.224	1.00	18.06
5767	CA	LEU	B	96	14.897	25.584	6.562	1.00	18.72
5769	CB	LEU	B	96	14.324	24.528	5.642	1.00	19.20
5772	CG	LEU	B	96	15.224	23.982	4.548	1.00	19.55
5774	CD1	LEU	B	96	14.392	23.084	3.642	1.00	21.29
5778	CD2	LEU	B	96	15.912	25.114	3.771	1.00	19.66
5782	C	LEU	B	96	13.814	26.018	7.551	1.00	18.78
5783	O	LEU	B	96	13.179	27.057	7.360	1.00	19.38
5784	N	ILE	B	97	13.607	25.227	8.599	1.00	18.35
5786	CA	ILE	B	97	12.581	25.536	9.612	1.00	18.39
5788	CB	ILE	B	97	12.525	24.456	10.724	1.00	18.49
5790	CG1	ILE	B	97	12.050	23.122	10.161	1.00	19.38
5793	CD1	ILE	B	97	12.339	21.950	11.075	1.00	20.40
5797	CG2	ILE	B	97	11.617	24.887	11.862	1.00	18.22
5801	C	ILE	B	97	12.874	26.891	10.247	1.00	18.35
5802	O	ILE	B	97	11.976	27.698	10.437	1.00	18.38
5803	N	HIS	B	98	14.142	27.127	10.568	1.00	18.85
5805	CA	HIS	B	98	14.554	28.377	11.204	1.00	18.52
5807	CB	HIS	B	98	15.891	28.199	11.898	1.00	19.08
5810	CG	HIS	B	98	15.787	27.494	13.204	1.00	18.65
5811	ND1	HIS	B	98	16.798	27.505	14.135	1.00	19.24
5813	CE1	HIS	B	98	16.422	26.803	15.188	1.00	20.04
5815	NE2	HIS	B	98	15.204	26.341	14.976	1.00	19.64
5817	CD2	HIS	B	98	14.785	26.756	13.738	1.00	20.54
5819	C	HIS	B	98	14.588	29.526	10.189	1.00	18.70
5820	O	HIS	B	98	14.261	30.658	10.527	1.00	18.65
5821	N	ASP	B	99	14.949	29.218	8.946	1.00	18.55
5823	CA	ASP	B	99	14.971	30.199	7.861	1.00	18.61
5825	CB	ASP	B	99	15.515	29.530	6.605	1.00	18.44
5828	CG	ASP	B	99	15.629	30.470	5.456	1.00	18.37
5829	OD1	ASP	B	99	14.710	30.462	4.590	1.00	16.28

FIGURE 3 (Cont.)CE

A	B	C	D	E	F	G	H	I	J
5830	OD2	ASP	B	99	16.618	31.233	5.324	1.00	20.63
5831	C	ASP	B	99	13.581	30.809	7.572	1.00	18.97
5832	O	ASP	B	99	13.471	31.985	7.256	1.00	19.10
5833	N	ASP	B	100	12.537	30.007	7.703	1.00	19.32
5835	CA	ASP	B	100	11.172	30.446	7.448	1.00	20.42
5837	CB	ASP	B	100	10.283	29.224	7.206	1.00	20.29
5840	CG	ASP	B	100	10.566	28.544	5.883	1.00	20.45
5841	OD1	ASP	B	100	10.363	27.303	5.791	1.00	21.30
5842	OD2	ASP	B	100	10.981	29.158	4.885	1.00	20.64
5843	C	ASP	B	100	10.524	31.287	8.577	1.00	20.97
5844	O	ASP	B	100	9.465	31.874	8.372	1.00	21.34
5845	N	LEU	B	101	11.150	31.332	9.748	1.00	21.55
5847	CA	LEU	B	101	10.588	31.991	10.925	1.00	22.27
5849	CB	LEU	B	101	11.551	31.861	12.120	1.00	22.07
5852	CG	LEU	B	101	11.746	30.451	12.684	1.00	22.57
5854	CD1	LEU	B	101	12.901	30.397	13.690	1.00	21.96
5858	CD2	LEU	B	101	10.471	29.947	13.317	1.00	23.63
5862	C	LEU	B	101	10.313	33.470	10.646	1.00	22.59
5863	O	LEU	B	101	11.025	34.078	9.870	1.00	22.10
5864	N	PRO	B	102	9.262	34.035	11.242	1.00	23.34
5865	CA	PRO	B	102	8.959	35.467	11.096	1.00	23.88
5867	CB	PRO	B	102	7.886	35.698	12.152	1.00	23.65
5870	CG	PRO	B	102	7.151	34.422	12.154	1.00	24.22
5873	CD	PRO	B	102	8.225	33.347	12.024	1.00	23.27
5876	C	PRO	B	102	10.131	36.428	11.282	1.00	24.08
5877	O	PRO	B	102	10.211	37.387	10.523	1.00	24.64
5878	N	ALA	B	103	11.019	36.183	12.243	1.00	24.21
5880	CA	ALA	B	103	12.179	37.054	12.450	1.00	24.56
5882	CB	ALA	B	103	12.804	36.795	13.823	1.00	24.65
5886	C	ALA	B	103	13.235	36.885	11.364	1.00	24.37
5887	O	ALA	B	103	14.092	37.756	11.188	1.00	25.00
5888	N	MET	B	104	13.193	35.747	10.674	1.00	23.93
5890	CA	MET	B	104	14.111	35.445	9.578	1.00	24.35
5892	CB	MET	B	104	14.527	33.969	9.642	1.00	24.14
5895	CG	MET	B	104	15.317	33.629	10.912	1.00	26.61
5898	SD	MET	B	104	17.063	34.058	10.820	1.00	29.08
5899	CE	MET	B	104	17.584	33.058	9.452	1.00	29.15
5903	C	MET	B	104	13.463	35.845	8.237	1.00	23.69
5904	O	MET	B	104	13.310	37.040	7.995	1.00	23.79
5905	N	ASP	B	105	13.044	34.885	7.404	1.00	23.23
5907	CA	ASP	B	105	12.489	35.198	6.073	1.00	22.98
5909	CB	ASP	B	105	12.936	34.167	5.016	1.00	22.62
5912	CG	ASP	B	105	14.429	34.138	4.838	1.00	21.61
5913	OD1	ASP	B	105	14.957	33.260	4.090	1.00	18.84
5914	OD2	ASP	B	105	15.163	34.963	5.413	1.00	21.22
5915	C	ASP	B	105	10.967	35.289	6.067	1.00	23.49
5916	O	ASP	B	105	10.365	35.645	5.054	1.00	22.75
5917	N	ASP	B	106	10.348	34.950	7.185	1.00	23.98
5919	CA	ASP	B	106	8.907	35.099	7.339	1.00	25.41
5921	CB	ASP	B	106	8.567	36.597	7.503	1.00	25.60
5924	CG	ASP	B	106	7.203	36.817	8.103	1.00	27.51
5925	OD1	ASP	B	106	6.682	37.941	7.973	1.00	29.77

FIGURE 3 ~~(Cont.)~~CF

A	B	C	D	E	F	G	H	I	J
5926	OD2	ASP	B	106	6.583	35.930	8.728	1.00	28.05
5927	C	ASP	B	106	8.126	34.503	6.172	1.00	25.57
5928	O	ASP	B	106	7.385	35.206	5.498	1.00	25.87
5929	N	ASP	B	107	8.309	33.203	5.936	1.00	26.04
5931	CA	ASP	B	107	7.630	32.487	4.861	1.00	25.95
5933	CB	ASP	B	107	8.641	31.685	4.032	1.00	26.04
5936	CG	ASP	B	107	9.212	32.477	2.895	1.00	26.93
5937	OD1	ASP	B	107	8.428	32.869	2.004	1.00	30.09
5938	OD2	ASP	B	107	10.426	32.755	2.786	1.00	25.96
5939	C	ASP	B	107	6.573	31.549	5.403	1.00	26.02
5940	O	ASP	B	107	6.773	30.883	6.425	1.00	26.50
5941	N	ASP	B	108	5.443	31.487	4.703	1.00	25.79
5943	CA	ASP	B	108	4.331	30.628	5.107	1.00	25.53
5945	CB	ASP	B	108	3.012	31.404	5.131	1.00	25.80
5948	CG	ASP	B	108	2.611	31.970	3.766	1.00	28.04
5949	OD1	ASP	B	108	1.460	32.426	3.651	1.00	30.10
5950	OD2	ASP	B	108	3.356	32.024	2.762	1.00	28.90
5951	C	ASP	B	108	4.183	29.359	4.260	1.00	24.50
5952	O	ASP	B	108	3.362	28.516	4.588	1.00	23.73
5953	N	LEU	B	109	4.975	29.228	3.197	1.00	23.97
5955	CA	LEU	B	109	4.939	28.054	2.323	1.00	23.69
5957	CB	LEU	B	109	4.386	28.414	0.940	1.00	24.10
5960	CG	LEU	B	109	2.907	28.201	0.569	1.00	27.09
5962	CD1	LEU	B	109	2.748	28.570	-0.917	1.00	27.23
5966	CD2	LEU	B	109	2.367	26.794	0.840	1.00	25.73
5970	C	LEU	B	109	6.329	27.462	2.103	1.00	22.98
5971	O	LEU	B	109	7.271	28.178	1.813	1.00	22.51
5972	N	ARG	B	110	6.426	26.146	2.208	1.00	22.68
5974	CA	ARG	B	110	7.609	25.422	1.776	1.00	22.37
5976	CB	ARG	B	110	8.662	25.359	2.878	1.00	22.08
5979	CG	ARG	B	110	9.916	24.624	2.441	1.00	21.74
5982	CD	ARG	B	110	11.021	24.622	3.487	1.00	19.15
5985	NE	ARG	B	110	11.586	25.949	3.737	1.00	17.98
5987	CZ	ARG	B	110	12.421	26.579	2.911	1.00	18.36
5988	NH1	ARG	B	110	12.900	27.771	3.239	1.00	19.16
5991	NH2	ARG	B	110	12.789	26.027	1.770	1.00	18.06
5994	C	ARG	B	110	7.210	24.022	1.382	1.00	22.36
5995	O	ARG	B	110	6.409	23.385	2.071	1.00	22.81
5996	N	ARG	B	111	7.789	23.549	0.283	1.00	22.18
5998	CA	ARG	B	111	7.542	22.212	-0.244	1.00	22.54
6000	CB	ARG	B	111	8.143	21.147	0.679	1.00	22.32
6003	CG	ARG	B	111	9.662	21.147	0.734	1.00	21.77
6006	CD	ARG	B	111	10.202	20.545	2.021	1.00	21.80
6009	NE	ARG	B	111	11.633	20.275	1.973	1.00	20.78
6011	CZ	ARG	B	111	12.305	19.671	2.947	1.00	20.45
6012	NH1	ARG	B	111	11.688	19.269	4.048	1.00	18.82
6015	NH2	ARG	B	111	13.608	19.464	2.826	1.00	19.98
6018	C	ARG	B	111	6.042	21.973	-0.465	1.00	23.08
6019	O	ARG	B	111	5.544	20.861	-0.338	1.00	22.39
6020	N	GLY	B	112	5.335	23.042	-0.807	1.00	23.92
6022	CA	GLY	B	112	3.921	22.975	-1.135	1.00	24.69
6025	C	GLY	B	112	3.010	23.023	0.070	1.00	24.98

FIGURE 3 ~~(Cont.)~~CG

A	B	C	D	E	F	G	H	I	J
6026	O	GLY	B	112	1.808	22.978	-0.089	1.00	25.54
6027	N	LEU	B	113	3.578	23.126	1.268	1.00	25.57
6029	CA	LEU	B	113	2.813	23.045	2.508	1.00	25.94
6031	CB	LEU	B	113	3.226	21.797	3.283	1.00	26.65
6034	CG	LEU	B	113	3.068	20.468	2.548	1.00	29.36
6036	CD1	LEU	B	113	3.750	19.369	3.338	1.00	31.10
6040	CD2	LEU	B	113	1.599	20.127	2.336	1.00	31.06
6044	C	LEU	B	113	3.043	24.272	3.388	1.00	25.32
6045	O	LEU	B	113	4.027	24.999	3.216	1.00	24.34
6046	N	PRO	B	114	2.153	24.497	4.355	1.00	25.34
6047	CA	PRO	B	114	2.425	25.500	5.383	1.00	24.92
6049	CB	PRO	B	114	1.261	25.331	6.348	1.00	25.42
6052	CG	PRO	B	114	0.165	24.734	5.503	1.00	25.33
6055	CD	PRO	B	114	0.862	23.812	4.575	1.00	25.09
6058	C	PRO	B	114	3.764	25.201	6.077	1.00	24.65
6059	O	PRO	B	114	4.051	24.057	6.403	1.00	24.29
6060	N	THR	B	115	4.583	26.222	6.259	1.00	24.42
6062	CA	THR	B	115	5.850	26.062	6.966	1.00	24.49
6064	CB	THR	B	115	6.635	27.364	6.990	1.00	24.32
6066	OG1	THR	B	115	5.798	28.437	7.465	1.00	26.32
6068	CG2	THR	B	115	7.058	27.773	5.573	1.00	24.50
6072	C	THR	B	115	5.607	25.577	8.387	1.00	24.50
6073	O	THR	B	115	4.512	25.721	8.944	1.00	23.20
6074	N	CYS	B	116	6.641	24.995	8.969	1.00	24.26
6076	CA	CYS	B	116	6.537	24.419	10.297	1.00	24.93
6078	CB	CYS	B	116	7.885	23.869	10.759	1.00	24.70
6081	SG	CYS	B	116	8.346	22.384	9.881	1.00	26.74
6082	C	CYS	B	116	6.002	25.412	11.305	1.00	24.67
6083	O	CYS	B	116	5.204	25.042	12.148	1.00	25.48
6084	N	HIS	B	117	6.408	26.672	11.212	1.00	24.78
6086	CA	HIS	B	117	5.981	27.647	12.214	1.00	25.04
6088	CB	HIS	B	117	6.888	28.867	12.233	1.00	25.27
6091	CG	HIS	B	117	6.649	29.828	11.116	1.00	25.24
6092	ND1	HIS	B	117	5.983	31.018	11.293	1.00	26.70
6094	CE1	HIS	B	117	5.924	31.663	10.141	1.00	27.42
6096	NE2	HIS	B	117	6.532	30.935	9.226	1.00	26.41
6098	CD2	HIS	B	117	6.985	29.776	9.807	1.00	26.27
6100	C	HIS	B	117	4.539	28.076	12.018	1.00	25.01
6101	O	HIS	B	117	3.891	28.466	12.971	1.00	25.49
6102	N	VAL	B	118	4.051	28.021	10.784	1.00	25.12
6104	CA	VAL	B	118	2.631	28.253	10.508	1.00	25.25
6106	CB	VAL	B	118	2.394	28.567	9.018	1.00	25.46
6108	CG1	VAL	B	118	0.884	28.609	8.673	1.00	26.21
6112	CG2	VAL	B	118	3.035	29.894	8.681	1.00	25.70
6116	C	VAL	B	118	1.786	27.078	10.999	1.00	25.08
6117	O	VAL	B	118	0.821	27.285	11.720	1.00	24.86
6118	N	LYS	B	119	2.167	25.856	10.639	1.00	25.25
6120	CA	LYS	B	119	1.439	24.654	11.042	1.00	25.87
6122	CB	LYS	B	119	1.935	23.428	10.263	1.00	26.25
6125	CG	LYS	B	119	0.884	22.726	9.418	1.00	28.80
6128	CD	LYS	B	119	-0.165	22.025	10.250	1.00	31.95
6131	CE	LYS	B	119	-0.978	21.015	9.432	1.00	33.31

FIGURE 3 (Cont.)CH

A	B	C	D	E	F	G	H	I	J
6134	NZ	LYS	B	119	-1.864	21.671	8.417	1.00	34.97
6138	C	LYS	B	119	1.468	24.365	12.564	1.00	25.31
6139	O	LYS	B	119	0.445	24.061	13.161	1.00	24.99
6140	N	PHE	B	120	2.626	24.488	13.193	1.00	24.69
6142	CA	PHE	B	120	2.789	24.032	14.567	1.00	24.30
6144	CB	PHE	B	120	3.908	22.993	14.616	1.00	24.16
6147	CG	PHE	B	120	3.639	21.763	13.799	1.00	24.65
6148	CD1	PHE	B	120	2.915	20.704	14.332	1.00	26.16
6150	CE1	PHE	B	120	2.690	19.541	13.582	1.00	25.66
6152	CZ	PHE	B	120	3.192	19.441	12.311	1.00	25.37
6154	CE2	PHE	B	120	3.930	20.494	11.767	1.00	24.54
6156	CD2	PHE	B	120	4.158	21.637	12.513	1.00	25.35
6158	C	PHE	B	120	3.084	25.165	15.565	1.00	23.77
6159	O	PHE	B	120	3.155	24.927	16.752	1.00	23.66
6160	N	GLY	B	121	3.250	26.391	15.083	1.00	23.69
6162	CA	GLY	B	121	3.622	27.516	15.935	1.00	23.51
6165	C	GLY	B	121	5.130	27.773	15.955	1.00	23.55
6166	O	GLY	B	121	5.927	26.892	15.652	1.00	22.34
6167	N	GLU	B	122	5.518	28.986	16.320	1.00	23.70
6169	CA	GLU	B	122	6.934	29.381	16.314	1.00	24.67
6171	CB	GLU	B	122	7.091	30.868	16.639	1.00	24.89
6174	CG	GLU	B	122	6.990	31.777	15.427	1.00	27.84
6177	CD	GLU	B	122	7.069	33.248	15.796	1.00	30.34
6178	OE1	GLU	B	122	8.174	33.721	16.136	1.00	35.10
6179	OE2	GLU	B	122	6.033	33.931	15.743	1.00	32.39
6180	C	GLU	B	122	7.792	28.558	17.283	1.00	24.12
6181	O	GLU	B	122	8.925	28.199	16.955	1.00	23.74
6182	N	ALA	B	123	7.249	28.292	18.469	1.00	23.52
6184	CA	ALA	B	123	7.968	27.587	19.526	1.00	23.88
6186	CB	ALA	B	123	7.156	27.594	20.816	1.00	23.93
6190	C	ALA	B	123	8.287	26.159	19.098	1.00	23.98
6191	O	ALA	B	123	9.417	25.688	19.247	1.00	22.97
6192	N	ASN	B	124	7.290	25.494	18.524	1.00	23.86
6194	CA	ASN	B	124	7.484	24.159	17.980	1.00	24.09
6196	CB	ASN	B	124	6.165	23.561	17.486	1.00	24.26
6199	CG	ASN	B	124	5.365	22.896	18.601	1.00	26.12
6200	OD1	ASN	B	124	4.125	22.946	18.602	1.00	27.70
6201	ND2	ASN	B	124	6.064	22.278	19.561	1.00	23.40
6204	C	ASN	B	124	8.508	24.168	16.849	1.00	23.11
6205	O	ASN	B	124	9.294	23.250	16.750	1.00	22.29
6206	N	ALA	B	125	8.496	25.208	16.015	1.00	22.58
6208	CA	ALA	B	125	9.430	25.303	14.896	1.00	22.31
6210	CB	ALA	B	125	9.043	26.425	13.953	1.00	23.02
6214	C	ALA	B	125	10.836	25.526	15.405	1.00	21.81
6215	O	ALA	B	125	11.766	24.906	14.932	1.00	21.37
6216	N	ILE	B	126	10.985	26.419	16.371	1.00	21.15
6218	CA	ILE	B	126	12.293	26.701	16.936	1.00	20.84
6220	CB	ILE	B	126	12.177	27.795	18.007	1.00	20.71
6222	CG1	ILE	B	126	11.994	29.168	17.339	1.00	21.50
6225	CD1	ILE	B	126	11.342	30.199	18.243	1.00	22.29
6229	CG2	ILE	B	126	13.395	27.816	18.903	1.00	21.11
6233	C	ILE	B	126	12.888	25.423	17.523	1.00	19.99

FIGURE 3 ~~(Cont.)~~<u>CI</u>

A	B	C	D	E	F	G	H	I	J
6234	O	ILE	B	126	14.037	25.072	17.234	1.00	19.91
6235	N	LEU	B	127	12.094	24.746	18.342	1.00	19.38
6237	CA	LEU	B	127	12.522	23.553	19.061	1.00	19.20
6239	CB	LEU	B	127	11.477	23.141	20.106	1.00	19.23
6242	CG	LEU	B	127	11.417	24.029	21.357	1.00	20.75
6244	CD1	LEU	B	127	12.776	24.131	22.047	1.00	22.13
6248	CD2	LEU	B	127	10.382	23.528	22.321	1.00	22.65
6252	C	LEU	B	127	12.776	22.413	18.096	1.00	19.26
6253	O	LEU	B	127	13.757	21.682	18.244	1.00	19.51
6254	N	ALA	B	128	11.926	22.286	17.082	1.00	18.61
6256	CA	ALA	B	128	12.073	21.218	16.108	1.00	19.13
6258	CB	ALA	B	128	10.873	21.183	15.181	1.00	18.64
6262	C	ALA	B	128	13.373	21.368	15.315	1.00	18.57
6263	O	ALA	B	128	14.079	20.387	15.065	1.00	18.99
6264	N	GLY	B	129	13.685	22.595	14.916	1.00	18.91
6266	CA	GLY	B	129	14.948	22.879	14.272	1.00	18.59
6269	C	GLY	B	129	16.117	22.574	15.200	1.00	18.99
6270	O	GLY	B	129	17.098	21.959	14.790	1.00	18.66
6271	N	ASP	B	130	16.001	22.986	16.459	1.00	19.11
6273	CA	ASP	B	130	17.061	22.771	17.457	1.00	19.02
6275	CB	ASP	B	130	16.652	23.327	18.829	1.00	18.48
6278	CG	ASP	B	130	16.654	24.851	18.881	1.00	20.10
6279	OD1	ASP	B	130	17.086	25.482	17.880	1.00	19.13
6280	OD2	ASP	B	130	16.221	25.488	19.889	1.00	20.44
6281	C	ASP	B	130	17.344	21.283	17.586	1.00	18.66
6282	O	ASP	B	130	18.481	20.860	17.541	1.00	18.36
6283	N	ALA	B	131	16.274	20.506	17.675	1.00	18.43
6285	CA	ALA	B	131	16.347	19.069	17.878	1.00	18.51
6287	CB	ALA	B	131	15.012	18.540	18.344	1.00	18.33
6291	C	ALA	B	131	16.808	18.315	16.629	1.00	18.44
6292	O	ALA	B	131	17.407	17.248	16.748	1.00	18.67
6293	N	LEU	B	132	16.518	18.850	15.445	1.00	18.17
6295	CA	LEU	B	132	16.970	18.235	14.207	1.00	18.20
6297	CB	LEU	B	132	16.213	18.786	12.995	1.00	18.38
6300	CG	LEU	B	132	14.853	18.138	12.732	1.00	17.74
6302	CD1	LEU	B	132	14.127	18.905	11.651	1.00	17.44
6306	CD2	LEU	B	132	15.017	16.674	12.341	1.00	18.02
6310	C	LEU	B	132	18.467	18.452	14.034	1.00	18.06
6311	O	LEU	B	132	19.167	17.572	13.544	1.00	18.16
6312	N	GLN	B	133	18.969	19.610	14.447	1.00	17.91
6314	CA	GLN	B	133	20.412	19.804	14.412	1.00	18.74
6316	CB	GLN	B	133	20.838	21.223	14.800	1.00	18.78
6319	CG	GLN	B	133	22.358	21.369	14.668	1.00	21.69
6322	CD	GLN	B	133	22.953	22.631	15.232	1.00	23.34
6323	OE1	GLN	B	133	22.274	23.644	15.458	1.00	24.32
6324	NE2	GLN	B	133	24.255	22.578	15.452	1.00	26.40
6327	C	GLN	B	133	21.094	18.762	15.319	1.00	18.33
6328	O	GLN	B	133	22.086	18.144	14.926	1.00	18.38
6329	N	THR	B	134	20.542	18.560	16.508	1.00	17.86
6331	CA	THR	B	134	21.121	17.657	17.476	1.00	18.15
6333	CB	THR	B	134	20.384	17.734	18.820	1.00	18.21
6335	OG1	THR	B	134	20.296	19.101	19.283	1.00	18.94

FIGURE 3 (Cont.)CJ

A	B	C	D	E	F	G	H	I	J
6337	CG2	THR	B	134	21.169	17.017	19.864	1.00	19.06
6341	C	THR	B	134	21.060	16.225	16.950	1.00	18.22
6342	O	THR	B	134	22.014	15.474	17.106	1.00	18.09
6343	N	LEU	B	135	19.936	15.870	16.322	1.00	17.83
6345	CA	LEU	B	135	19.739	14.530	15.781	1.00	17.43
6347	CB	LEU	B	135	18.336	14.416	15.184	1.00	17.61
6350	CG	LEU	B	135	18.006	13.113	14.455	1.00	18.78
6352	CD1	LEU	B	135	18.167	11.908	15.367	1.00	18.23
6356	CD2	LEU	B	135	16.619	13.201	13.912	1.00	19.31
6360	C	LEU	B	135	20.818	14.186	14.743	1.00	16.77
6361	O	LEU	B	135	21.287	13.045	14.664	1.00	16.01
6362	N	ALA	B	136	21.243	15.179	13.970	1.00	16.82
6364	CA	ALA	B	136	22.280	14.960	12.974	1.00	16.89
6366	CB	ALA	B	136	22.581	16.241	12.231	1.00	17.47
6370	C	ALA	B	136	23.548	14.406	13.625	1.00	17.27
6371	O	ALA	B	136	24.184	13.484	13.091	1.00	17.46
6372	N	PHE	B	137	23.888	14.943	14.789	1.00	17.08
6374	CA	PHE	B	137	25.088	14.528	15.496	1.00	17.65
6376	CB	PHE	B	137	25.593	15.666	16.381	1.00	18.03
6379	CG	PHE	B	137	26.007	16.880	15.584	1.00	18.67
6380	CD1	PHE	B	137	25.230	18.019	15.566	1.00	18.86
6382	CE1	PHE	B	137	25.605	19.122	14.809	1.00	19.97
6384	CZ	PHE	B	137	26.757	19.070	14.029	1.00	19.23
6386	CE2	PHE	B	137	27.526	17.940	14.023	1.00	19.82
6388	CD2	PHE	B	137	27.140	16.835	14.788	1.00	21.06
6390	C	PHE	B	137	24.848	13.218	16.260	1.00	17.89
6391	O	PHE	B	137	25.764	12.440	16.419	1.00	17.92
6392	N	SER	B	138	23.613	12.966	16.699	1.00	18.09
6394	CA	SER	B	138	23.275	11.661	17.269	1.00	18.71
6396	CB	SER	B	138	21.839	11.634	17.769	1.00	18.28
6399	OG	SER	B	138	21.712	12.386	18.950	1.00	19.32
6401	C	SER	B	138	23.466	10.571	16.212	1.00	18.94
6402	O	SER	B	138	24.084	9.555	16.485	1.00	19.25
6403	N	ILE	B	139	22.967	10.819	15.001	1.00	19.22
6405	CA	ILE	B	139	23.123	9.884	13.890	1.00	19.25
6407	CB	ILE	B	139	22.430	10.403	12.622	1.00	19.39
6409	CG1	ILE	B	139	20.916	10.363	12.822	1.00	18.95
6412	CD1	ILE	B	139	20.144	11.100	11.805	1.00	21.43
6416	CG2	ILE	B	139	22.848	9.571	11.387	1.00	17.88
6420	C	ILE	B	139	24.606	9.609	13.612	1.00	19.87
6421	O	ILE	B	139	25.021	8.461	13.593	1.00	19.68
6422	N	LEU	B	140	25.397	10.648	13.393	1.00	19.88
6424	CA	LEU	B	140	26.799	10.451	13.025	1.00	20.40
6426	CB	LEU	B	140	27.452	11.764	12.620	1.00	20.25
6429	CG	LEU	B	140	27.071	12.298	11.246	1.00	20.51
6431	CD1	LEU	B	140	27.798	13.593	11.005	1.00	23.24
6435	CD2	LEU	B	140	27.402	11.299	10.149	1.00	21.98
6439	C	LEU	B	140	27.600	9.803	14.145	1.00	20.89
6440	O	LEU	B	140	28.572	9.088	13.876	1.00	21.00
6441	N	SER	B	141	27.211	10.045	15.396	1.00	21.26
6443	CA	SER	B	141	27.933	9.439	16.514	1.00	22.16
6445	CB	SER	B	141	27.926	10.329	17.756	1.00	21.93

FIGURE 3 (Cont.)CK

A	B	C	D	E	F	G	H	I	J
6448	OG	SER	B	141	26.615	10.552	18.225	1.00	23.99
6450	C	SER	B	141	27.456	8.023	16.856	1.00	22.90
6451	O	SER	B	141	28.248	7.250	17.390	1.00	22.85
6452	N	ASP	B	142	26.203	7.678	16.538	1.00	23.91
6454	CA	ASP	B	142	25.580	6.411	16.991	1.00	24.85
6456	CB	ASP	B	142	24.270	6.674	17.745	1.00	25.39
6459	CG	ASP	B	142	24.464	7.509	18.995	1.00	26.64
6460	OD1	ASP	B	142	23.535	8.249	19.365	1.00	25.98
6461	OD2	ASP	B	142	25.516	7.497	19.667	1.00	29.60
6462	C	ASP	B	142	25.262	5.407	15.890	1.00	25.42
6463	O	ASP	B	142	25.185	4.202	16.158	1.00	25.21
6464	N	ALA	B	143	25.052	5.887	14.663	1.00	25.69
6466	CA	ALA	B	143	24.533	5.031	13.592	1.00	26.20
6468	CB	ALA	B	143	24.187	5.840	12.367	1.00	26.13
6472	C	ALA	B	143	25.542	3.965	13.226	1.00	26.52
6473	O	ALA	B	143	26.739	4.190	13.292	1.00	26.08
6474	N	ASP	B	144	25.051	2.790	12.862	1.00	27.00
6476	CA	ASP	B	144	25.908	1.760	12.308	1.00	27.79
6478	CB	ASP	B	144	25.084	0.487	12.088	1.00	28.61
6481	CG	ASP	B	144	25.935	-0.733	11.853	1.00	30.23
6482	OD1	ASP	B	144	27.147	-0.714	12.160	1.00	33.26
6483	OD2	ASP	B	144	25.452	-1.776	11.358	1.00	34.68
6484	C	ASP	B	144	26.531	2.247	10.992	1.00	27.76
6485	O	ASP	B	144	25.825	2.652	10.050	1.00	27.93
6486	N	MET	B	145	27.856	2.247	10.951	1.00	27.25
6488	CA	MET	B	145	28.612	2.526	9.743	1.00	27.33
6490	CB	MET	B	145	29.181	3.936	9.772	1.00	26.88
6493	CG	MET	B	145	28.129	5.014	9.664	1.00	26.79
6496	SD	MET	B	145	28.859	6.646	9.270	1.00	27.26
6497	CE	MET	B	145	29.830	6.916	10.701	1.00	23.05
6501	C	MET	B	145	29.737	1.508	9.657	1.00	27.62
6502	O	MET	B	145	30.895	1.812	9.936	1.00	26.26
6503	N	PRO	B	146	29.393	0.291	9.256	1.00	28.79
6504	CA	PRO	B	146	30.354	-0.815	9.234	1.00	29.73
6506	CB	PRO	B	146	29.669	-1.832	8.320	1.00	29.99
6509	CG	PRO	B	146	28.228	-1.630	8.593	1.00	29.30
6512	CD	PRO	B	146	28.060	-0.137	8.799	1.00	29.11
6515	C	PRO	B	146	31.733	-0.464	8.696	1.00	30.46
6516	O	PRO	B	146	32.732	-0.822	9.317	1.00	30.83
6517	N	GLU	B	147	31.801	0.253	7.586	1.00	31.81
6519	CA	GLU	B	147	33.089	0.431	6.905	1.00	33.36
6521	CB	GLU	B	147	32.889	0.840	5.426	1.00	34.57
6524	CG	GLU	B	147	31.629	0.304	4.730	1.00	37.40
6527	CD	GLU	B	147	31.768	0.264	3.209	1.00	41.76
6528	OE1	GLU	B	147	30.918	-0.387	2.543	1.00	42.19
6529	OE2	GLU	B	147	32.733	0.877	2.676	1.00	43.49
6530	C	GLU	B	147	34.030	1.449	7.587	1.00	32.65
6531	O	GLU	B	147	35.172	1.605	7.155	1.00	33.17
6532	N	VAL	B	148	33.572	2.099	8.660	1.00	31.25
6534	CA	VAL	B	148	34.097	3.410	9.043	1.00	30.18
6536	CB	VAL	B	148	32.970	4.456	9.012	1.00	30.21
6538	CG1	VAL	B	148	33.501	5.842	9.381	1.00	29.95

FIGURE 3 (Cont.)CL

A	B	C	D	E	F	G	H	I	J
6542	CG2	VAL	B	148	32.310	4.467	7.634	1.00	30.63
6546	C	VAL	B	148	34.767	3.425	10.417	1.00	28.89
6547	O	VAL	B	148	34.131	3.174	11.431	1.00	27.43
6548	N	SER	B	149	36.057	3.755	10.435	1.00	28.02
6550	CA	SER	B	149	36.806	3.836	11.681	1.00	27.32
6552	CB	SER	B	149	38.302	4.022	11.413	1.00	27.23
6555	OG	SER	B	149	38.554	5.276	10.811	1.00	25.67
6557	C	SER	B	149	36.295	4.984	12.540	1.00	27.03
6558	O	SER	B	149	35.651	5.906	12.045	1.00	26.50
6559	N	ASP	B	150	36.601	4.899	13.831	1.00	26.71
6561	CA	ASP	B	150	36.236	5.914	14.810	1.00	26.65
6563	CB	ASP	B	150	36.729	5.509	16.194	1.00	26.35
6566	CG	ASP	B	150	35.776	4.575	16.906	1.00	28.03
6567	OD1	ASP	B	150	36.086	4.216	18.054	1.00	30.17
6568	OD2	ASP	B	150	34.692	4.157	16.424	1.00	29.62
6569	C	ASP	B	150	36.824	7.253	14.407	1.00	26.23
6570	O	ASP	B	150	36.146	8.269	14.454	1.00	25.29
6571	N	ARG	B	151	38.077	7.229	13.970	1.00	26.28
6573	CA	ARG	B	151	38.745	8.409	13.442	1.00	26.55
6575	CB	ARG	B	151	40.172	8.069	13.019	1.00	27.45
6578	CG	ARG	B	151	41.099	9.254	13.054	1.00	30.78
6581	CD	ARG	B	151	41.726	9.500	14.416	1.00	34.73
6584	NE	ARG	B	151	41.001	10.520	15.179	1.00	38.97
6586	CZ	ARG	B	151	41.152	11.835	15.043	1.00	42.64
6587	NH1	ARG	B	151	42.000	12.354	14.148	1.00	45.06
6590	NH2	ARG	B	151	40.435	12.651	15.801	1.00	43.15
6593	C	ARG	B	151	38.004	9.052	12.268	1.00	25.50
6594	O	ARG	B	151	37.870	10.265	12.211	1.00	25.19
6595	N	ASP	B	152	37.540	8.252	11.315	1.00	24.83
6597	CA	ASP	B	152	36.823	8.813	10.171	1.00	24.18
6599	CB	ASP	B	152	36.747	7.809	9.030	1.00	24.78
6602	CG	ASP	B	152	38.117	7.499	8.443	1.00	26.32
6603	OD1	ASP	B	152	39.074	8.280	8.679	1.00	29.38
6604	OD2	ASP	B	152	38.329	6.479	7.758	1.00	28.43
6605	C	ASP	B	152	35.427	9.290	10.562	1.00	22.75
6606	O	ASP	B	152	34.923	10.240	10.007	1.00	22.39
6607	N	ARG	B	153	34.810	8.619	11.521	1.00	21.86
6609	CA	ARG	B	153	33.532	9.053	12.064	1.00	20.79
6611	CB	ARG	B	153	33.022	8.054	13.088	1.00	20.74
6614	CG	ARG	B	153	31.647	8.375	13.651	1.00	20.82
6617	CD	ARG	B	153	31.205	7.399	14.704	1.00	20.94
6620	NE	ARG	B	153	30.980	6.045	14.173	1.00	22.48
6622	CZ	ARG	B	153	29.790	5.511	13.895	1.00	23.71
6623	NH1	ARG	B	153	29.723	4.256	13.448	1.00	25.23
6626	NH2	ARG	B	153	28.671	6.205	14.046	1.00	20.67
6629	C	ARG	B	153	33.676	10.426	12.714	1.00	20.58
6630	O	ARG	B	153	32.833	11.297	12.519	1.00	18.98
6631	N	ILE	B	154	34.752	10.610	13.483	1.00	20.29
6633	CA	ILE	B	154	35.016	11.891	14.124	1.00	20.38
6635	CB	ILE	B	154	36.209	11.808	15.090	1.00	20.21
6637	CG1	ILE	B	154	35.848	10.962	16.319	1.00	20.02
6640	CD1	ILE	B	154	37.077	10.390	17.035	1.00	21.78

FIGURE 3 (Cont.)CM

A	B	C	D	E	F	G	H	I	J
6644	CG2	ILE	B	154	36.656	13.203	15.514	1.00	21.46
6648	C	ILE	B	154	35.247	12.940	13.051	1.00	20.53
6649	O	ILE	B	154	34.737	14.018	13.158	1.00	20.41
6650	N	SER	B	155	35.976	12.593	11.996	1.00	21.07
6652	CA	SER	B	155	36.182	13.485	10.864	1.00	21.78
6654	CB	SER	B	155	37.097	12.822	9.824	1.00	22.36
6657	OG	SER	B	155	38.452	13.117	10.107	1.00	25.91
6659	C	SER	B	155	34.867	13.924	10.186	1.00	21.46
6660	O	SER	B	155	34.771	15.053	9.711	1.00	21.56
6661	N	MET	B	156	33.886	13.029	10.125	1.00	21.47
6663	CA	MET	B	156	32.569	13.337	9.576	1.00	21.23
6665	CB	MET	B	156	31.726	12.079	9.403	1.00	21.94
6668	CG	MET	B	156	32.183	11.183	8.281	1.00	24.79
6671	SD	MET	B	156	31.189	9.677	8.224	1.00	31.73
6672	CE	MET	B	156	32.337	8.674	7.553	1.00	32.04
6676	C	MET	B	156	31.815	14.278	10.480	1.00	20.18
6677	O	MET	B	156	31.164	15.191	10.005	1.00	20.12
6678	N	ILE	B	157	31.894	14.045	11.782	1.00	20.00
6680	CA	ILE	B	157	31.238	14.915	12.744	1.00	19.69
6682	CB	ILE	B	157	31.290	14.326	14.178	1.00	19.62
6684	CG1	ILE	B	157	30.466	13.047	14.259	1.00	19.47
6687	CD1	ILE	B	157	30.741	12.182	15.483	1.00	21.29
6691	CG2	ILE	B	157	30.763	15.332	15.177	1.00	18.69
6695	C	ILE	B	157	31.878	16.289	12.688	1.00	19.80
6696	O	ILE	B	157	31.182	17.300	12.684	1.00	20.00
6697	N	SER	B	158	33.204	16.340	12.640	1.00	19.73
6699	CA	SER	B	158	33.894	17.619	12.559	1.00	19.44
6701	CB	SER	B	158	35.410	17.419	12.507	1.00	19.53
6704	OG	SER	B	158	36.053	18.665	12.347	1.00	19.74
6706	C	SER	B	158	33.469	18.403	11.325	1.00	19.46
6707	O	SER	B	158	33.193	19.587	11.408	1.00	18.61
6708	N	GLU	B	159	33.429	17.734	10.181	1.00	20.02
6710	CA	GLU	B	159	33.084	18.384	8.932	1.00	20.06
6712	CB	GLU	B	159	33.224	17.423	7.757	1.00	20.49
6715	CG	GLU	B	159	32.576	17.922	6.472	1.00	21.89
6718	CD	GLU	B	159	33.103	19.290	6.041	1.00	23.61
6719	OE1	GLU	B	159	34.281	19.584	6.322	1.00	24.99
6720	OE2	GLU	B	159	32.347	20.067	5.426	1.00	25.28
6721	C	GLU	B	159	31.658	18.934	8.990	1.00	19.72
6722	O	GLU	B	159	31.422	20.062	8.577	1.00	19.69
6723	N	LEU	B	160	30.720	18.140	9.494	1.00	18.90
6725	CA	LEU	B	160	29.324	18.550	9.526	1.00	18.94
6727	CB	LEU	B	160	28.406	17.404	9.956	1.00	18.87
6730	CG	LEU	B	160	26.915	17.695	9.771	1.00	19.53
6732	CD1	LEU	B	160	26.644	18.166	8.357	1.00	19.83
6736	CD2	LEU	B	160	26.076	16.470	10.093	1.00	20.63
6740	C	LEU	B	160	29.158	19.736	10.458	1.00	18.48
6741	O	LEU	B	160	28.486	20.694	10.130	1.00	18.99
6742	N	ALA	B	161	29.803	19.673	11.612	1.00	18.69
6744	CA	ALA	B	161	29.769	20.773	12.560	1.00	18.51
6746	CB	ALA	B	161	30.446	20.384	13.872	1.00	18.21
6750	C	ALA	B	161	30.377	22.045	11.970	1.00	19.04

FIGURE 3 ~~(Cont.)~~<u>CN</u>

A	B	C	D	E	F	G	H	I	J
6751	O	ALA	B	161	29.749	23.095	12.012	1.00	18.97
6752	N	SER	B	162	31.573	21.976	11.387	1.00	19.49
6754	CA	SER	B	162	32.161	23.190	10.838	1.00	19.97
6756	CB	SER	B	162	33.630	22.988	10.472	1.00	20.60
6759	OG	SER	B	162	33.756	21.975	9.518	1.00	24.18
6761	C	SER	B	162	31.348	23.734	9.643	1.00	19.40
6762	O	SER	B	162	31.186	24.958	9.482	1.00	18.70
6763	N	ALA	B	163	30.813	22.832	8.825	1.00	19.19
6765	CA	ALA	B	163	29.974	23.225	7.690	1.00	18.98
6767	CB	ALA	B	163	29.671	22.011	6.798	1.00	19.19
6771	C	ALA	B	163	28.672	23.907	8.081	1.00	18.85
6772	O	ALA	B	163	28.157	24.742	7.341	1.00	19.30
6773	N	SER	B	164	28.135	23.537	9.228	1.00	18.81
6775	CA	SER	B	164	26.788	23.931	9.638	1.00	18.52
6777	CB	SER	B	164	26.128	22.787	10.405	1.00	18.45
6780	OG	SER	B	164	26.073	21.610	9.622	1.00	18.06
6782	C	SER	B	164	26.780	25.159	10.526	1.00	18.48
6783	O	SER	B	164	25.779	25.828	10.630	1.00	18.20
6784	N	GLY	B	165	27.902	25.438	11.177	1.00	19.42
6786	CA	GLY	B	165	27.950	26.481	12.175	1.00	19.70
6789	C	GLY	B	165	28.359	27.810	11.598	1.00	20.33
6790	O	GLY	B	165	28.096	28.122	10.441	1.00	19.41
6791	N	ILE	B	166	29.018	28.604	12.424	1.00	21.45
6793	CA	ILE	B	166	29.348	29.976	12.074	1.00	22.91
6795	CB	ILE	B	166	29.846	30.707	13.354	1.00	23.50
6797	CG1	ILE	B	166	29.737	32.206	13.173	1.00	25.77
6800	CD1	ILE	B	166	28.314	32.688	13.353	1.00	25.49
6804	CG2	ILE	B	166	31.229	30.245	13.727	1.00	24.89
6808	C	ILE	B	166	30.354	30.068	10.916	1.00	22.56
6809	O	ILE	B	166	30.335	31.016	10.141	1.00	22.77
6810	N	ALA	B	167	31.207	29.059	10.771	1.00	22.49
6812	CA	ALA	B	167	32.152	29.006	9.656	1.00	22.06
6814	CB	ALA	B	167	33.324	28.148	10.023	1.00	21.92
6818	C	ALA	B	167	31.490	28.488	8.383	1.00	22.04
6819	O	ALA	B	167	32.146	28.318	7.376	1.00	22.97
6820	N	GLY	B	168	30.181	28.252	8.430	1.00	21.24
6822	CA	GLY	B	168	29.464	27.684	7.313	1.00	20.53
6825	C	GLY	B	168	28.034	28.189	7.292	1.00	20.28
6826	O	GLY	B	168	27.804	29.394	7.295	1.00	19.03
6827	N	MET	B	169	27.082	27.265	7.340	1.00	20.39
6829	CA	MET	B	169	25.676	27.559	7.077	1.00	21.14
6831	CB	MET	B	169	24.855	26.298	7.278	1.00	21.40
6834	CG	MET	B	169	23.410	26.392	6.837	1.00	23.14
6837	SD	MET	B	169	22.401	27.153	8.090	1.00	26.74
6838	CE	MET	B	169	22.407	25.862	9.410	1.00	26.17
6842	C	MET	B	169	25.147	28.696	7.938	1.00	21.67
6843	O	MET	B	169	24.556	29.644	7.436	1.00	21.21
6844	N	CYS	B	170	25.367	28.594	9.239	1.00	22.13
6846	CA	CYS	B	170	24.827	29.556	10.170	1.00	22.50
6848	CB	BCYS	B	170	25.042	29.096	11.614	0.35	22.49
6849	CB	ACYS	B	170	25.010	29.057	11.596	0.65	22.96
6854	SG	BCYS	B	170	23.609	28.307	12.340	0.35	22.05

FIGURE 3 ~~(Cont.)~~CO

A	B	C	D	E	F	G	H	I	J
6855	SG	ACYS	B	170	24.028	29.996	12.749	0.65	25.42
6856	C	CYS	B	170	25.460	30.935	9.997	1.00	21.94
6857	O	CYS	B	170	24.775	31.934	10.105	1.00	22.08
6858	N	GLY	B	171	26.767	30.980	9.758	1.00	21.27
6860	CA	GLY	B	171	27.453	32.231	9.504	1.00	21.35
6863	C	GLY	B	171	26.951	32.858	8.218	1.00	20.97
6864	O	GLY	B	171	26.839	34.081	8.111	1.00	20.81
6865	N	GLY	B	172	26.643	32.009	7.249	1.00	20.08
6867	CA	GLY	B	172	26.027	32.440	6.009	1.00	19.62
6870	C	GLY	B	172	24.641	33.007	6.215	1.00	19.25
6871	O	GLY	B	172	24.288	34.011	5.605	1.00	18.27
6872	N	GLN	B	173	23.858	32.380	7.084	1.00	18.75
6874	CA	GLN	B	173	22.535	32.890	7.404	1.00	19.22
6876	CB	GLN	B	173	21.787	31.947	8.348	1.00	19.67
6879	CG	GLN	B	173	21.349	30.652	7.682	1.00	20.18
6882	CD	GLN	B	173	20.333	30.899	6.597	1.00	20.92
6883	OE1	GLN	B	173	20.701	31.297	5.496	1.00	21.77
6884	NE2	GLN	B	173	19.047	30.712	6.914	1.00	19.90
6887	C	GLN	B	173	22.632	34.281	8.002	1.00	19.31
6888	O	GLN	B	173	21.805	35.146	7.691	1.00	18.98
6889	N	ALA	B	174	23.667	34.503	8.810	1.00	19.26
6891	CA	ALA	B	174	23.894	35.813	9.437	1.00	20.09
6893	CB	ALA	B	174	24.956	35.725	10.526	1.00	19.57
6897	C	ALA	B	174	24.292	36.845	8.387	1.00	20.47
6898	O	ALA	B	174	23.826	37.969	8.440	1.00	21.60
6899	N	LEU	B	175	25.143	36.464	7.436	1.00	21.00
6901	CA	LEU	B	175	25.561	37.384	6.371	1.00	21.21
6903	CB	LEU	B	175	26.646	36.753	5.497	1.00	21.41
6906	CG	LEU	B	175	28.026	36.557	6.121	1.00	23.45
6908	CD1	LEU	B	175	28.948	35.855	5.138	1.00	24.47
6912	CD2	LEU	B	175	28.630	37.913	6.562	1.00	24.78
6916	C	LEU	B	175	24.358	37.776	5.519	1.00	21.36
6917	O	LEU	B	175	24.210	38.942	5.118	1.00	20.88
6918	N	ASP	B	176	23.498	36.794	5.258	1.00	21.82
6920	CA	ASP	B	176	22.291	36.980	4.466	1.00	22.30
6922	CB	ASP	B	176	21.615	35.625	4.252	1.00	22.47
6925	CG	ASP	B	176	20.205	35.739	3.779	1.00	21.57
6926	OD1	ASP	B	176	19.938	35.449	2.588	1.00	22.94
6927	OD2	ASP	B	176	19.281	36.072	4.540	1.00	25.04
6928	C	ASP	B	176	21.356	37.989	5.138	1.00	23.38
6929	O	ASP	B	176	20.856	38.927	4.499	1.00	23.61
6930	N	LEU	B	177	21.131	37.814	6.429	1.00	24.61
6932	CA	LEU	B	177	20.296	38.751	7.181	1.00	26.08
6934	CB	LEU	B	177	20.112	38.267	8.621	1.00	26.86
6937	CG	LEU	B	177	18.842	37.475	8.968	1.00	28.65
6939	CD1	LEU	B	177	18.029	36.990	7.768	1.00	30.94
6943	CD2	LEU	B	177	19.243	36.330	9.825	1.00	29.29
6947	C	LEU	B	177	20.891	40.147	7.193	1.00	26.38
6948	O	LEU	B	177	20.176	41.134	7.048	1.00	27.18
6949	N	ASP	B	178	22.203	40.228	7.355	1.00	27.07
6951	CA	ASP	B	178	22.893	41.513	7.389	1.00	27.97
6953	CB	ASP	B	178	24.336	41.337	7.864	1.00	28.49

FIGURE 3 (Cont.)CP

A	B	C	D	E	F	G	H	I	J
6956	CG	ASP	B	178	24.926	42.624	8.427	1.00	31.55
6957	OD1	ASP	B	178	25.937	43.106	7.874	1.00	34.43
6958	OD2	ASP	B	178	24.447	43.218	9.419	1.00	36.43
6959	C	ASP	B	178	22.865	42.228	6.034	1.00	27.98
6960	O	ASP	B	178	22.853	43.454	5.993	1.00	27.47
6961	N	ALA	B	179	22.828	41.462	4.936	1.00	27.64
6963	CA	ALA	B	179	22.818	42.026	3.576	1.00	27.64
6965	CB	ALA	B	179	23.397	41.024	2.579	1.00	27.26
6969	C	ALA	B	179	21.415	42.474	3.118	1.00	27.90
6970	O	ALA	B	179	21.288	43.142	2.109	1.00	27.38
6971	N	GLU	B	180	20.374	42.097	3.852	1.00	28.50
6973	CA	GLU	B	180	19.006	42.515	3.535	1.00	29.13
6975	CB	GLU	B	180	18.031	42.069	4.629	1.00	29.71
6978	CG	GLU	B	180	17.071	40.969	4.234	1.00	31.66
6981	CD	GLU	B	180	16.175	40.534	5.384	1.00	33.14
6982	OE1	GLU	B	180	15.509	41.400	5.995	1.00	35.30
6983	OE2	GLU	B	180	16.149	39.324	5.684	1.00	32.62
6984	C	GLU	B	180	18.922	44.041	3.418	1.00	29.49
6985	O	GLU	B	180	19.290	44.755	4.348	1.00	28.60
6986	N	GLY	B	181	18.454	44.518	2.264	1.00	29.61
6988	CA	GLY	B	181	18.279	45.935	1.997	1.00	29.83
6991	C	GLY	B	181	19.560	46.670	1.658	1.00	30.04
6992	O	GLY	B	181	19.532	47.871	1.420	1.00	30.48
6993	N	LYS	B	182	20.681	45.954	1.622	1.00	30.21
6995	CA	LYS	B	182	21.992	46.573	1.506	1.00	30.46
6997	CB	LYS	B	182	22.959	45.982	2.526	1.00	30.97
7000	CG	LYS	B	182	22.593	46.287	3.973	1.00	32.58
7003	CD	LYS	B	182	23.830	46.343	4.864	1.00	34.32
7006	CE	LYS	B	182	23.490	46.882	6.259	1.00	35.98
7009	NZ	LYS	B	182	23.339	45.804	7.290	1.00	36.88
7013	C	LYS	B	182	22.573	46.427	0.116	1.00	30.22
7014	O	LYS	B	182	23.559	47.083	-0.203	1.00	30.23
7015	N	HIS	B	183	21.984	45.555	-0.700	1.00	29.28
7017	CA	HIS	B	183	22.375	45.441	-2.093	1.00	29.34
7019	CB	HIS	B	183	21.892	46.684	-2.856	1.00	29.70
7022	CG	HIS	B	183	20.410	46.833	-2.832	1.00	30.08
7023	ND1	HIS	B	183	19.699	47.003	-1.668	1.00	32.28
7025	CE1	HIS	B	183	18.412	47.068	-1.942	1.00	31.16
7027	NE2	HIS	B	183	18.261	46.940	-3.244	1.00	32.50
7029	CD2	HIS	B	183	19.497	46.782	-3.821	1.00	32.70
7031	C	HIS	B	183	23.887	45.297	-2.191	1.00	28.93
7032	O	HIS	B	183	24.558	46.097	-2.847	1.00	29.19
7033	N	VAL	B	184	24.415	44.274	-1.522	1.00	27.85
7035	CA	VAL	B	184	25.850	44.103	-1.417	1.00	27.29
7037	CB	VAL	B	184	26.247	43.065	-0.319	1.00	27.33
7039	CG1	VAL	B	184	25.636	43.452	1.052	1.00	27.10
7043	CG2	VAL	B	184	25.860	41.634	-0.722	1.00	27.05
7047	C	VAL	B	184	26.419	43.723	-2.779	1.00	26.86
7048	O	VAL	B	184	25.733	43.075	-3.577	1.00	26.12
7049	N	PRO	B	185	27.663	44.126	-3.051	1.00	26.31
7050	CA	PRO	B	185	28.314	43.792	-4.319	1.00	26.16
7052	CB	PRO	B	185	29.596	44.623	-4.284	1.00	26.24

FIGURE 3 (Cont.)CQ

A	B	C	D	E	F	G	H	I	J
7055	CG	PRO	B	185	29.892	44.801	-2.835	1.00	26.65
7058	CD	PRO	B	185	28.552	44.905	-2.168	1.00	26.81
7061	C	PRO	B	185	28.646	42.297	-4.436	1.00	25.85
7062	O	PRO	B	185	28.521	41.553	-3.475	1.00	24.67
7063	N	LEU	B	186	29.106	41.908	-5.616	1.00	26.22
7065	CA	LEU	B	186	29.284	40.509	-6.002	1.00	26.42
7067	CB	LEU	B	186	29.859	40.422	-7.424	1.00	26.65
7070	CG	LEU	B	186	29.462	39.279	-8.371	1.00	28.07
7072	CD1	LEU	B	186	30.565	39.033	-9.399	1.00	29.61
7076	CD2	LEU	B	186	29.105	38.004	-7.671	1.00	28.33
7080	C	LEU	B	186	30.183	39.726	-5.048	1.00	26.27
7081	O	LEU	B	186	29.890	38.580	-4.737	1.00	25.80
7082	N	ASP	B	187	31.286	40.317	-4.590	1.00	26.90
7084	CA	ASP	B	187	32.198	39.558	-3.721	1.00	27.11
7086	CB	ASP	B	187	33.567	40.236	-3.526	1.00	27.85
7089	CG	ASP	B	187	33.480	41.648	-2.951	1.00	30.82
7090	OD1	ASP	B	187	34.555	42.173	-2.574	1.00	36.51
7091	OD2	ASP	B	187	32.435	42.331	-2.848	1.00	35.53
7092	C	ASP	B	187	31.554	39.180	-2.380	1.00	26.24
7093	O	ASP	B	187	31.729	38.053	-1.900	1.00	25.65
7094	N	ALA	B	188	30.809	40.117	-1.799	1.00	25.42
7096	CA	ALA	B	188	30.097	39.892	-0.548	1.00	24.85
7098	CB	ALA	B	188	29.610	41.221	0.019	1.00	24.84
7102	C	ALA	B	188	28.915	38.951	-0.774	1.00	24.38
7103	O	ALA	B	188	28.578	38.154	0.081	1.00	24.14
7104	N	LEU	B	189	28.291	39.059	-1.942	1.00	24.33
7106	CA	LEU	B	189	27.156	38.230	-2.286	1.00	24.42
7108	CB	LEU	B	189	26.530	38.741	-3.577	1.00	24.99
7111	CG	LEU	B	189	25.509	37.865	-4.268	1.00	25.94
7113	CD1	LEU	B	189	24.317	37.593	-3.350	1.00	26.65
7117	CD2	LEU	B	189	25.072	38.566	-5.566	1.00	26.30
7121	C	LEU	B	189	27.607	36.783	-2.435	1.00	23.85
7122	O	LEU	B	189	26.965	35.863	-1.918	1.00	23.56
7123	N	GLU	B	190	28.727	36.590	-3.115	1.00	23.22
7125	CA	GLU	B	190	29.301	35.269	-3.280	1.00	23.29
7127	CB	GLU	B	190	30.566	35.331	-4.135	1.00	23.75
7130	CG	GLU	B	190	31.070	33.963	-4.535	1.00	25.63
7133	CD	GLU	B	190	32.356	33.994	-5.339	1.00	28.46
7134	OE1	GLU	B	190	33.201	33.121	-5.090	1.00	31.64
7135	OE2	GLU	B	190	32.522	34.854	-6.226	1.00	32.12
7136	C	GLU	B	190	29.625	34.655	-1.917	1.00	22.85
7137	O	GLU	B	190	29.434	33.459	-1.699	1.00	20.62
7138	N	ARG	B	191	30.114	35.490	-1.009	1.00	22.57
7140	CA	ARG	B	191	30.499	35.041	0.315	1.00	22.97
7142	CB	ARG	B	191	31.169	36.171	1.077	1.00	23.59
7145	CG	ARG	B	191	31.646	35.789	2.444	1.00	26.56
7148	CD	ARG	B	191	32.707	36.714	3.004	1.00	31.42
7151	NE	ARG	B	191	32.158	37.666	3.962	1.00	35.82
7153	CZ	ARG	B	191	32.874	38.304	4.891	1.00	38.83
7154	NH1	ARG	B	191	34.184	38.105	5.012	1.00	39.90
7157	NH2	ARG	B	191	32.270	39.150	5.712	1.00	40.92
7160	C	ARG	B	191	29.282	34.546	1.087	1.00	21.94

FIGURE 3 (Cont.)CR

A	B	C	D	E	F	G	H	I	J
7161	O	ARG	B	191	29.357	33.536	1.770	1.00	22.24
7162	N	ILE	B	192	28.160	35.246	0.947	1.00	21.11
7164	CA	ILE	B	192	26.916	34.836	1.574	1.00	19.99
7166	CB	ILE	B	192	25.763	35.775	1.186	1.00	19.92
7168	CG1	ILE	B	192	25.925	37.151	1.835	1.00	20.88
7171	CD1	ILE	B	192	25.092	38.196	1.195	1.00	21.97
7175	CG2	ILE	B	192	24.408	35.196	1.598	1.00	19.49
7179	C	ILE	B	192	26.589	33.421	1.107	1.00	19.95
7180	O	ILE	B	192	26.387	32.538	1.914	1.00	19.48
7181	N	HIS	B	193	26.542	33.231	-0.207	1.00	19.56
7183	CA	HIS	B	193	26.027	31.999	-0.802	1.00	18.94
7185	CB	HIS	B	193	25.801	32.209	-2.298	1.00	19.11
7188	CG	HIS	B	193	24.584	33.024	-2.606	1.00	17.67
7189	ND1	HIS	B	193	23.920	33.755	-1.647	1.00	19.83
7191	CE1	HIS	B	193	22.873	34.349	-2.191	1.00	19.06
7193	NE2	HIS	B	193	22.821	34.013	-3.467	1.00	19.16
7195	CD2	HIS	B	193	23.882	33.186	-3.754	1.00	19.39
7197	C	HIS	B	193	26.913	30.802	-0.543	1.00	18.45
7198	O	HIS	B	193	26.422	29.700	-0.294	1.00	18.16
7199	N	ARG	B	194	28.221	31.017	-0.579	1.00	18.21
7201	CA	ARG	B	194	29.157	29.954	-0.301	1.00	18.14
7203	CB	ARG	B	194	30.582	30.396	-0.588	1.00	18.28
7206	CG	ARG	B	194	30.894	30.549	-2.059	1.00	18.14
7209	CD	ARG	B	194	32.368	30.534	-2.332	1.00	19.86
7212	NE	ARG	B	194	32.685	30.696	-3.740	1.00	20.51
7214	CZ	ARG	B	194	32.656	29.723	-4.648	1.00	23.08
7215	NH1	ARG	B	194	32.326	28.482	-4.320	1.00	24.68
7218	NH2	ARG	B	194	32.981	29.995	-5.900	1.00	25.18
7221	C	ARG	B	194	29.003	29.465	1.143	1.00	18.28
7222	O	ARG	B	194	29.037	28.267	1.392	1.00	18.15
7223	N	HIS	B	195	28.782	30.390	2.079	1.00	18.49
7225	CA	HIS	B	195	28.558	30.036	3.479	1.00	18.76
7227	CB	HIS	B	195	28.786	31.251	4.390	1.00	18.80
7230	CG	HIS	B	195	30.224	31.612	4.533	1.00	19.89
7231	ND1	HIS	B	195	30.934	32.241	3.533	1.00	21.51
7233	CE1	HIS	B	195	32.186	32.408	3.925	1.00	21.57
7235	NE2	HIS	B	195	32.311	31.910	5.142	1.00	21.37
7237	CD2	HIS	B	195	31.103	31.395	5.541	1.00	21.40
7239	C	HIS	B	195	27.170	29.430	3.697	1.00	18.88
7240	O	HIS	B	195	27.050	28.298	4.182	1.00	19.41
7241	N	LYS	B	196	26.117	30.122	3.293	1.00	18.32
7243	CA	LYS	B	196	24.778	29.672	3.686	1.00	18.29
7245	CB	LYS	B	196	23.725	30.764	3.506	1.00	18.11
7248	CG	LYS	B	196	23.241	31.027	2.080	1.00	17.45
7251	CD	LYS	B	196	22.081	32.049	2.131	1.00	17.15
7254	CE	LYS	B	196	21.634	32.547	0.768	1.00	15.61
7257	NZ	LYS	B	196	20.235	33.122	0.794	1.00	15.01
7261	C	LYS	B	196	24.322	28.389	3.006	1.00	18.44
7262	O	LYS	B	196	23.466	27.688	3.541	1.00	18.43
7263	N	THR	B	197	24.898	28.098	1.841	1.00	17.92
7265	CA	THR	B	197	24.454	27.009	0.983	1.00	18.22
7267	CB	THR	B	197	23.686	27.598	-0.203	1.00	17.81

FIGURE 3 ~~(Cont.)~~CS

A	B	C	D	E	F	G	H	I	J
7269	OG1	THR	B	197	22.429	28.070	0.261	1.00	18.26
7271	CG2	THR	B	197	23.322	26.539	-1.246	1.00	18.58
7275	C	THR	B	197	25.601	26.129	0.504	1.00	17.84
7276	O	THR	B	197	25.482	24.907	0.475	1.00	18.55
7277	N	GLY	B	198	26.703	26.746	0.104	1.00	17.60
7279	CA	GLY	B	198	27.854	26.006	-0.358	1.00	17.04
7282	C	GLY	B	198	28.469	25.112	0.708	1.00	16.72
7283	O	GLY	B	198	28.863	23.993	0.415	1.00	15.65
7284	N	ALA	B	199	28.523	25.581	1.951	1.00	16.19
7286	CA	ALA	B	199	29.239	24.837	2.993	1.00	16.23
7288	CB	ALA	B	199	29.265	25.611	4.271	1.00	16.00
7292	C	ALA	B	199	28.633	23.441	3.200	1.00	16.09
7293	O	ALA	B	199	29.357	22.445	3.312	1.00	16.00
7294	N	LEU	B	200	27.309	23.363	3.200	1.00	15.80
7296	CA	LEU	B	200	26.623	22.126	3.536	1.00	16.20
7298	CB	LEU	B	200	25.202	22.408	4.018	1.00	16.05
7301	CG	LEU	B	200	24.363	21.238	4.540	1.00	18.16
7303	CD1	LEU	B	200	25.019	20.573	5.727	1.00	18.85
7307	CD2	LEU	B	200	22.989	21.735	4.928	1.00	18.03
7311	C	LEU	B	200	26.593	21.206	2.332	1.00	16.19
7312	O	LEU	B	200	26.544	19.993	2.479	1.00	15.79
7313	N	ILE	B	201	26.615	21.769	1.136	1.00	16.74
7315	CA	ILE	B	201	26.723	20.928	-0.052	1.00	17.10
7317	CB	ILE	B	201	26.341	21.713	-1.305	1.00	17.41
7319	CG1	ILE	B	201	24.806	21.764	-1.403	1.00	18.09
7322	CD1	ILE	B	201	24.283	22.985	-2.120	1.00	19.65
7326	CG2	ILE	B	201	26.936	21.073	-2.581	1.00	16.41
7330	C	ILE	B	201	28.130	20.312	-0.110	1.00	17.27
7331	O	ILE	B	201	28.289	19.126	-0.436	1.00	16.47
7332	N	ARG	B	202	29.139	21.098	0.240	1.00	17.03
7334	CA	ARG	B	202	30.468	20.539	0.389	1.00	17.33
7336	CB	ARG	B	202	31.516	21.598	0.645	1.00	17.65
7339	CG	ARG	B	202	32.956	20.997	0.625	1.00	18.08
7342	CD	ARG	B	202	34.038	22.029	0.637	1.00	19.46
7345	NE	ARG	B	202	33.985	22.829	1.854	1.00	21.33
7347	CZ	ARG	B	202	34.772	23.882	2.089	1.00	22.51
7348	NH1	ARG	B	202	34.662	24.547	3.222	1.00	23.90
7351	NH2	ARG	B	202	35.663	24.271	1.199	1.00	21.54
7354	C	ARG	B	202	30.517	19.475	1.475	1.00	17.44
7355	O	ARG	B	202	31.179	18.451	1.295	1.00	17.53
7356	N	ALA	B	203	29.804	19.689	2.580	1.00	17.13
7358	CA	ALA	B	203	29.776	18.709	3.658	1.00	16.93
7360	CB	ALA	B	203	28.967	19.200	4.832	1.00	17.56
7364	C	ALA	B	203	29.211	17.389	3.179	1.00	17.03
7365	O	ALA	B	203	29.704	16.351	3.574	1.00	15.70
7366	N	ALA	B	204	28.154	17.439	2.368	1.00	16.79
7368	CA	ALA	B	204	27.548	16.224	1.799	1.00	17.41
7370	CB	ALA	B	204	26.386	16.572	0.915	1.00	17.51
7374	C	ALA	B	204	28.560	15.419	1.002	1.00	17.70
7375	O	ALA	B	204	28.698	14.197	1.200	1.00	17.88
7376	N	VAL	B	205	29.268	16.107	0.109	1.00	17.07
7378	CA	VAL	B	205	30.282	15.471	-0.724	1.00	17.54

FIGURE 3 (Cont.)CT

A	B	C	D	E	F	G	H	I	J
7380	CB	VAL	B	205	30.849	16.429	-1.793	1.00	17.01
7382	CG1	VAL	B	205	31.962	15.769	-2.607	1.00	17.61
7386	CG2	VAL	B	205	29.750	16.884	-2.730	1.00	17.80
7390	C	VAL	B	205	31.400	14.924	0.150	1.00	18.04
7391	O	VAL	B	205	31.802	13.766	-0.005	1.00	17.71
7392	N	ARG	B	206	31.887	15.748	1.078	1.00	18.26
7394	CA	ARG	B	206	32.974	15.348	1.963	1.00	18.54
7396	CB	ARG	B	206	33.393	16.497	2.878	1.00	19.04
7399	CG	ARG	B	206	34.211	17.532	2.179	1.00	18.96
7402	CD	ARG	B	206	34.665	18.637	3.113	1.00	20.46
7405	NE	ARG	B	206	35.712	19.448	2.531	1.00	20.99
7407	CZ	ARG	B	206	36.218	20.545	3.102	1.00	21.01
7408	NH1	ARG	B	206	35.771	20.974	4.275	1.00	20.38
7411	NH2	ARG	B	206	37.190	21.204	2.495	1.00	20.62
7414	C	ARG	B	206	32.582	14.152	2.795	1.00	18.87
7415	O	ARG	B	206	33.368	13.219	2.935	1.00	18.67
7416	N	LEU	B	207	31.346	14.136	3.289	1.00	19.33
7418	CA	LEU	B	207	30.896	13.036	4.141	1.00	20.12
7420	CB	LEU	B	207	29.516	13.310	4.738	1.00	19.99
7423	CG	LEU	B	207	29.431	13.776	6.203	1.00	22.44
7425	CD1	LEU	B	207	30.464	14.770	6.559	1.00	24.69
7429	CD2	LEU	B	207	28.046	14.364	6.440	1.00	24.61
7433	C	LEU	B	207	30.887	11.715	3.370	1.00	20.21
7434	O	LEU	B	207	31.247	10.668	3.922	1.00	20.74
7435	N	GLY	B	208	30.461	11.750	2.110	1.00	20.90
7437	CA	GLY	B	208	30.546	10.578	1.246	1.00	21.11
7440	C	GLY	B	208	31.979	10.097	1.066	1.00	21.83
7441	O	GLY	B	208	32.263	8.898	1.152	1.00	22.91
7442	N	ALA	B	209	32.892	11.029	0.821	1.00	21.98
7444	CA	ALA	B	209	34.292	10.688	0.627	1.00	22.48
7446	CB	ALA	B	209	35.059	11.868	0.052	1.00	22.44
7450	C	ALA	B	209	34.934	10.189	1.928	1.00	23.19
7451	O	ALA	B	209	35.703	9.232	1.906	1.00	23.21
7452	N	LEU	B	210	34.582	10.804	3.058	1.00	23.38
7454	CA	LEU	B	210	35.144	10.429	4.355	1.00	23.77
7456	CB	LEU	B	210	34.733	11.429	5.440	1.00	23.69
7459	CG	LEU	B	210	35.459	12.768	5.355	1.00	23.52
7461	CD1	LEU	B	210	34.830	13.745	6.336	1.00	22.14
7465	CD2	LEU	B	210	36.962	12.569	5.630	1.00	24.32
7469	C	LEU	B	210	34.721	9.031	4.780	1.00	24.42
7470	O	LEU	B	210	35.379	8.410	5.603	1.00	24.38
7471	N	SER	B	211	33.627	8.541	4.211	1.00	25.75
7473	CA	SER	B	211	33.176	7.180	4.458	1.00	26.29
7475	CB	BSER	B	211	31.724	6.990	3.992	0.35	26.33
7476	CB	ASER	B	211	31.733	7.003	3.960	0.65	26.73
7481	OG	BSER	B	211	31.635	6.814	2.589	0.35	25.17
7482	OG	ASER	B	211	30.884	8.043	4.437	0.65	28.22
7485	C	SER	B	211	34.096	6.146	3.779	1.00	26.79
7486	O	SER	B	211	33.943	4.960	4.011	1.00	27.11
7487	N	ALA	B	212	35.052	6.609	2.971	1.00	27.48
7489	CA	ALA	B	212	35.807	5.765	2.045	1.00	28.00
7491	CB	ALA	B	212	35.502	6.200	0.610	1.00	27.64

FIGURE 3 (Cont.)CU

A	B	C	D	E	F	G	H	I	J
7495	C	ALA	B	212	37.330	5.735	2.259	1.00	28.36
7496	O	ALA	B	212	38.075	5.478	1.305	1.00	28.63
7497	N	GLY	B	213	37.793	6.017	3.480	1.00	28.63
7499	CA	GLY	B	213	39.190	5.812	3.848	1.00	28.66
7502	C	GLY	B	213	40.160	6.623	3.013	1.00	29.30
7503	O	GLY	B	213	39.829	7.754	2.628	1.00	29.18
7504	N	ASP	B	214	41.337	6.047	2.725	1.00	29.91
7506	CA	ASP	B	214	42.401	6.716	1.945	1.00	30.40
7508	CB	ASP	B	214	43.629	5.798	1.749	1.00	31.13
7511	CG	ASP	B	214	44.248	5.315	3.055	1.00	32.74
7512	OD1	ASP	B	214	44.060	5.963	4.113	1.00	34.47
7513	OD2	ASP	B	214	44.958	4.280	3.097	1.00	35.20
7514	C	ASP	B	214	41.960	7.157	0.541	1.00	30.05
7515	O	ASP	B	214	42.333	8.224	0.068	1.00	29.72
7516	N	LYS	B	215	41.203	6.319	-0.150	1.00	30.05
7518	CA	LYS	B	215	40.854	6.614	-1.546	1.00	29.92
7520	CB	LYS	B	215	40.230	5.391	-2.199	1.00	30.71
7523	CG	LYS	B	215	40.214	5.394	-3.723	1.00	32.45
7526	CD	LYS	B	215	39.887	3.980	-4.222	1.00	34.64
7529	CE	LYS	B	215	39.790	3.882	-5.732	1.00	36.80
7532	NZ	LYS	B	215	39.315	2.521	-6.190	1.00	38.07
7536	C	LYS	B	215	39.906	7.821	-1.634	1.00	28.89
7537	O	LYS	B	215	40.045	8.661	-2.525	1.00	28.45
7538	N	GLY	B	216	38.972	7.902	-0.689	1.00	27.81
7540	CA	GLY	B	216	38.049	9.018	-0.591	1.00	27.11
7543	C	GLY	B	216	38.781	10.292	-0.243	1.00	26.53
7544	O	GLY	B	216	38.559	11.333	-0.840	1.00	26.52
7545	N	ARG	B	217	39.690	10.198	0.720	1.00	26.28
7547	CA	ARG	B	217	40.519	11.340	1.099	1.00	25.74
7549	CB	ARG	B	217	41.263	11.018	2.393	1.00	25.35
7552	CG	ARG	B	217	40.332	11.005	3.598	1.00	28.38
7555	CD	ARG	B	217	40.945	10.453	4.857	1.00	31.47
7558	NE	ARG	B	217	40.208	10.787	6.078	1.00	33.37
7560	CZ	ARG	B	217	40.258	11.974	6.697	1.00	36.00
7561	NH1	ARG	B	217	40.977	12.979	6.200	1.00	39.28
7564	NH2	ARG	B	217	39.575	12.170	7.810	1.00	34.96
7567	C	ARG	B	217	41.471	11.800	-0.027	1.00	24.69
7568	O	ARG	B	217	41.743	12.983	-0.161	1.00	24.52
7569	N	ARG	B	218	41.956	10.873	-0.844	1.00	24.21
7571	CA	ARG	B	218	42.809	11.210	-1.983	1.00	23.79
7573	CB	ARG	B	218	43.340	9.927	-2.637	1.00	24.37
7576	CG	ARG	B	218	44.257	10.097	-3.872	1.00	27.47
7579	CD	ARG	B	218	43.908	9.115	-5.003	1.00	32.66
7582	NE	ARG	B	218	45.013	8.799	-5.908	1.00	36.58
7584	CZ	ARG	B	218	45.406	9.552	-6.933	1.00	39.40
7585	NH1	ARG	B	218	46.425	9.145	-7.688	1.00	40.57
7588	NH2	ARG	B	218	44.809	10.714	-7.204	1.00	39.74
7591	C	ARG	B	218	42.025	12.047	-3.005	1.00	22.91
7592	O	ARG	B	218	42.599	12.928	-3.640	1.00	22.18
7593	N	ALA	B	219	40.726	11.759	-3.149	1.00	21.70
7595	CA	ALA	B	219	39.845	12.476	-4.066	1.00	21.49
7597	CB	ALA	B	219	38.667	11.618	-4.422	1.00	21.35

FIGURE 3 (Cont.)CV

A	B	C	D	E	F	G	H	I	J
7601	C	ALA	B	219	39.340	13.818	-3.523	1.00	21.64
7602	O	ALA	B	219	38.756	14.587	-4.270	1.00	20.84
7603	N	LEU	B	220	39.563	14.090	-2.240	1.00	21.58
7605	CA	LEU	B	220	39.003	15.285	-1.600	1.00	22.20
7607	CB	LEU	B	220	39.340	15.335	-0.110	1.00	22.43
7610	CG	LEU	B	220	38.407	14.580	0.840	1.00	22.95
7612	CD1	LEU	B	220	38.991	14.642	2.244	1.00	24.14
7616	CD2	LEU	B	220	37.002	15.153	0.810	1.00	24.62
7620	C	LEU	B	220	39.364	16.616	-2.239	1.00	21.85
7621	O	LEU	B	220	38.482	17.438	-2.393	1.00	22.54
7622	N	PRO	B	221	40.627	16.872	-2.583	1.00	22.19
7623	CA	PRO	B	221	40.969	18.150	-3.227	1.00	22.28
7625	CB	PRO	B	221	42.442	17.987	-3.589	1.00	22.39
7628	CG	PRO	B	221	42.951	16.960	-2.616	1.00	23.34
7631	CD	PRO	B	221	41.812	16.025	-2.379	1.00	22.27
7634	C	PRO	B	221	40.115	18.420	-4.460	1.00	21.79
7635	O	PRO	B	221	39.580	19.513	-4.592	1.00	21.54
7636	N	VAL	B	222	39.945	17.431	-5.331	1.00	21.34
7638	CA	VAL	B	222	39.131	17.616	-6.533	1.00	20.96
7640	CB	VAL	B	222	39.431	16.533	-7.601	1.00	21.09
7642	CG1	VAL	B	222	38.492	16.664	-8.787	1.00	20.79
7646	CG2	VAL	B	222	40.885	16.668	-8.085	1.00	22.50
7650	C	VAL	B	222	37.620	17.635	-6.214	1.00	20.48
7651	O	VAL	B	222	36.877	18.411	-6.804	1.00	20.29
7652	N	LEU	B	223	37.172	16.773	-5.307	1.00	20.17
7654	CA	LEU	B	223	35.750	16.717	-4.924	1.00	19.91
7656	CB	LEU	B	223	35.466	15.562	-3.957	1.00	20.52
7659	CG	LEU	B	223	35.293	14.173	-4.587	1.00	21.95
7661	CD1	LEU	B	223	35.296	13.095	-3.512	1.00	22.04
7665	CD2	LEU	B	223	34.039	14.111	-5.407	1.00	23.07
7669	C	LEU	B	223	35.327	18.015	-4.253	1.00	19.72
7670	O	LEU	B	223	34.188	18.456	-4.381	1.00	19.07
7671	N	ASP	B	224	36.250	18.599	-3.503	1.00	19.68
7673	CA	ASP	B	224	36.042	19.893	-2.883	1.00	19.94
7675	CB	ASP	B	224	37.272	20.287	-2.069	1.00	19.86
7678	CG	ASP	B	224	37.289	19.671	-0.705	1.00	22.67
7679	OD1	ASP	B	224	36.256	19.094	-0.288	1.00	23.35
7680	OD2	ASP	B	224	38.304	19.744	0.036	1.00	25.14
7681	C	ASP	B	224	35.778	20.972	-3.908	1.00	19.81
7682	O	ASP	B	224	34.910	21.795	-3.702	1.00	19.95
7683	N	LYS	B	225	36.541	20.990	-4.996	1.00	19.94
7685	CA	LYS	B	225	36.368	22.027	-6.013	1.00	20.31
7687	CB	LYS	B	225	37.525	22.048	-7.022	1.00	20.63
7690	CG	LYS	B	225	38.973	22.184	-6.439	1.00	22.72
7693	CD	BLYS	B	225	39.100	23.053	-5.155	0.35	21.46
7694	CD	ALYS	B	225	39.001	22.753	-5.014	0.65	25.09
7699	CE	BLYS	B	225	39.223	22.270	-3.837	0.35	19.92
7700	CE	ALYS	B	225	39.871	23.974	-4.801	0.65	25.51
7705	NZ	BLYS	B	225	40.570	21.728	-3.502	0.35	14.63
7706	NZ	ALYS	B	225	39.377	24.575	-3.546	0.65	24.29
7713	C	LYS	B	225	35.049	21.804	-6.718	1.00	19.81
7714	O	LYS	B	225	34.320	22.762	-6.982	1.00	19.64

FIGURE 3 ~~(Cont.)~~<u>CW</u>

A	B	C	D	E	F	G	H	I	J
7715	N	TYR	B	226	34.733	20.536	-6.979	1.00	19.10
7717	CA	TYR	B	226	33.437	20.151	-7.525	1.00	18.47
7719	CB	TYR	B	226	33.307	18.624	-7.646	1.00	18.62
7722	CG	TYR	B	226	31.883	18.168	-7.875	1.00	17.81
7723	CD1	TYR	B	226	31.300	18.256	-9.132	1.00	17.52
7725	CE1	TYR	B	226	29.994	17.859	-9.337	1.00	20.05
7727	CZ	TYR	B	226	29.232	17.374	-8.279	1.00	18.47
7728	OH	TYR	B	226	27.919	16.982	-8.500	1.00	17.52
7730	CE2	TYR	B	226	29.785	17.299	-7.026	1.00	17.57
7732	CD2	TYR	B	226	31.112	17.694	-6.829	1.00	17.49
7734	C	TYR	B	226	32.331	20.699	-6.643	1.00	18.41
7735	O	TYR	B	226	31.452	21.411	-7.122	1.00	18.11
7736	N	ALA	B	227	32.417	20.408	-5.345	1.00	18.13
7738	CA	ALA	B	227	31.403	20.799	-4.377	1.00	18.18
7740	CB	ALA	B	227	31.723	20.221	-3.021	1.00	17.94
7744	C	ALA	B	227	31.281	22.316	-4.251	1.00	18.61
7745	O	ALA	B	227	30.196	22.851	-4.063	1.00	18.11
7746	N	GLU	B	228	32.407	22.996	-4.328	1.00	19.06
7748	CA	GLU	B	228	32.418	24.439	-4.177	1.00	20.24
7750	CB	GLU	B	228	33.864	24.949	-4.123	1.00	20.64
7753	CG	GLU	B	228	34.451	24.809	-2.730	1.00	23.29
7756	CD	GLU	B	228	35.947	24.586	-2.731	1.00	26.70
7757	OE1	GLU	B	228	36.464	23.942	-1.768	1.00	29.92
7758	OE2	GLU	B	228	36.592	25.044	-3.686	1.00	27.85
7759	C	GLU	B	228	31.636	25.080	-5.300	1.00	20.03
7760	O	GLU	B	228	30.842	25.982	-5.063	1.00	20.42
7761	N	SER	B	229	31.824	24.584	-6.521	1.00	20.10
7763	CA	SER	B	229	31.140	25.146	-7.663	1.00	20.21
7765	CB	SER	B	229	31.838	24.755	-8.958	1.00	20.74
7768	OG	SER	B	229	33.134	25.319	-8.986	1.00	21.81
7770	C	SER	B	229	29.655	24.795	-7.704	1.00	19.69
7771	O	SER	B	229	28.845	25.675	-7.972	1.00	19.58
7772	N	ILE	B	230	29.283	23.538	-7.451	1.00	19.26
7774	CA	ILE	B	230	27.855	23.173	-7.467	1.00	19.00
7776	CB	ILE	B	230	27.588	21.634	-7.493	1.00	19.39
7778	CG1	ILE	B	230	28.132	20.922	-6.249	1.00	19.42
7781	CD1	ILE	B	230	27.348	19.661	-5.883	1.00	19.21
7785	CG2	ILE	B	230	28.145	20.996	-8.778	1.00	20.74
7789	C	ILE	B	230	27.118	23.798	-6.292	1.00	18.75
7790	O	ILE	B	230	25.934	24.062	-6.404	1.00	18.69
7791	N	GLY	B	231	27.825	24.000	-5.179	1.00	17.92
7793	CA	GLY	B	231	27.260	24.588	-3.977	1.00	18.54
7796	C	GLY	B	231	26.885	26.044	-4.189	1.00	18.41
7797	O	GLY	B	231	25.776	26.467	-3.838	1.00	18.39
7798	N	LEU	B	232	27.791	26.809	-4.801	1.00	18.03
7800	CA	LEU	B	232	27.463	28.191	-5.176	1.00	17.92
7802	CB	LEU	B	232	28.697	28.973	-5.644	1.00	17.76
7805	CG	LEU	B	232	28.471	30.416	-6.137	1.00	18.58
7807	CD1	LEU	B	232	27.676	31.245	-5.123	1.00	20.10
7811	CD2	LEU	B	232	29.783	31.085	-6.471	1.00	19.77
7815	C	LEU	B	232	26.371	28.184	-6.232	1.00	17.69
7816	O	LEU	B	232	25.391	28.929	-6.125	1.00	17.69

FIGURE 3 (Cont.)CX

A	B	C	D	E	F	G	H	I	J
7817	N	ALA	B	233	26.520	27.332	-7.243	1.00	17.54
7819	CA	ALA	B	233	25.535	27.255	-8.330	1.00	17.52
7821	CB	ALA	B	233	25.937	26.175	-9.322	1.00	17.72
7825	C	ALA	B	233	24.133	26.996	-7.801	1.00	16.87
7826	O	ALA	B	233	23.149	27.503	-8.321	1.00	16.72
7827	N	PHE	B	234	24.055	26.207	-6.738	1.00	17.20
7829	CA	PHE	B	234	22.796	25.770	-6.175	1.00	17.20
7831	CB	PHE	B	234	23.077	24.798	-5.020	1.00	17.86
7834	CG	PHE	B	234	21.913	23.952	-4.635	1.00	19.19
7835	CD1	PHE	B	234	21.908	22.595	-4.939	1.00	23.96
7837	CE1	PHE	B	234	20.833	21.786	-4.576	1.00	25.08
7839	CZ	PHE	B	234	19.753	22.346	-3.895	1.00	23.44
7841	CE2	PHE	B	234	19.766	23.705	-3.578	1.00	21.13
7843	CD2	PHE	B	234	20.837	24.489	-3.936	1.00	19.81
7845	C	PHE	B	234	22.023	26.972	-5.659	1.00	17.12
7846	O	PHE	B	234	20.817	27.075	-5.856	1.00	16.09
7847	N	GLN	B	235	22.724	27.860	-4.969	1.00	16.71
7849	CA	GLN	B	235	22.093	29.040	-4.427	1.00	17.18
7851	CB	GLN	B	235	22.918	29.661	-3.304	1.00	16.88
7854	CG	GLN	B	235	22.173	30.781	-2.566	1.00	16.78
7857	CD	GLN	B	235	20.856	30.332	-1.970	1.00	18.18
7858	OE1	GLN	B	235	20.783	29.271	-1.353	1.00	17.96
7859	NE2	GLN	B	235	19.818	31.140	-2.138	1.00	15.32
7862	C	GLN	B	235	21.821	30.089	-5.501	1.00	16.98
7863	O	GLN	B	235	20.842	30.800	-5.392	1.00	16.15
7864	N	VAL	B	236	22.640	30.184	-6.544	1.00	17.46
7866	CA	VAL	B	236	22.265	31.160	-7.590	1.00	18.23
7868	CB	VAL	B	236	23.405	31.708	-8.547	1.00	18.68
7870	CG1	VAL	B	236	24.747	31.119	-8.271	1.00	19.87
7874	CG2	VAL	B	236	23.019	31.733	-10.030	1.00	19.70
7878	C	VAL	B	236	21.003	30.665	-8.279	1.00	17.45
7879	O	VAL	B	236	20.139	31.457	-8.531	1.00	17.04
7880	N	GLN	B	237	20.856	29.350	-8.447	1.00	17.88
7882	CA	GLN	B	237	19.649	28.785	-9.035	1.00	18.28
7884	CB	GLN	B	237	19.783	27.288	-9.337	1.00	18.86
7887	CG	GLN	B	237	18.561	26.715	-10.056	1.00	20.61
7890	CD	GLN	B	237	18.402	27.211	-11.478	1.00	23.91
7891	OE1	GLN	B	237	19.207	27.995	-11.962	1.00	27.71
7892	NE2	GLN	B	237	17.361	26.738	-12.157	1.00	25.53
7895	C	GLN	B	237	18.469	29.005	-8.135	1.00	17.68
7896	O	GLN	B	237	17.381	29.326	-8.612	1.00	18.18
7897	N	ASP	B	238	18.673	28.830	-6.832	1.00	16.95
7899	CA	ASP	B	238	17.624	29.133	-5.872	1.00	16.59
7901	CB	ASP	B	238	18.084	28.803	-4.452	1.00	15.86
7904	CG	ASP	B	238	16.988	28.976	-3.451	1.00	16.32
7905	OD1	ASP	B	238	16.037	28.162	-3.445	1.00	17.49
7906	OD2	ASP	B	238	16.959	29.929	-2.651	1.00	18.97
7907	C	ASP	B	238	17.186	30.610	-5.985	1.00	16.34
7908	O	ASP	B	238	16.001	30.905	-5.932	1.00	15.59
7909	N	ASP	B	239	18.135	31.526	-6.146	1.00	17.76
7911	CA	ASP	B	239	17.799	32.959	-6.321	1.00	18.83
7913	CB	ASP	B	239	19.044	33.819	-6.384	1.00	19.28

FIGURE 3 (Cont.)CY

A	B	C	D	E	F	G	H	I	J
7916	CG	ASP	B	239	19.766	33.928	-5.070	1.00	19.95
7917	OD1	ASP	B	239	19.251	33.447	-4.018	1.00	23.46
7918	OD2	ASP	B	239	20.886	34.480	-5.016	1.00	19.63
7919	C	ASP	B	239	17.021	33.192	-7.610	1.00	19.87
7920	O	ASP	B	239	16.020	33.917	-7.629	1.00	20.25
7921	N	ILE	B	240	17.492	32.570	-8.687	1.00	19.96
7923	CA	ILE	B	240	16.845	32.676	-9.986	1.00	20.61
7925	CB	ILE	B	240	17.647	31.902	-11.039	1.00	20.77
7927	CG1	ILE	B	240	18.945	32.645	-11.363	1.00	20.81
7930	CD1	ILE	B	240	19.974	31.792	-11.997	1.00	21.71
7934	CG2	ILE	B	240	16.821	31.682	-12.304	1.00	21.31
7938	C	ILE	B	240	15.413	32.161	-9.932	1.00	20.80
7939	O	ILE	B	240	14.506	32.784	-10.482	1.00	20.05
7940	N	LEU	B	241	15.214	31.014	-9.283	1.00	21.23
7942	CA	LEU	B	241	13.904	30.394	-9.206	1.00	21.82
7944	CB	LEU	B	241	14.009	28.986	-8.620	1.00	22.08
7947	CG	LEU	B	241	14.569	27.953	-9.600	1.00	23.04
7949	CD1	LEU	B	241	14.635	26.592	-8.926	1.00	25.03
7953	CD2	LEU	B	241	13.740	27.874	-10.869	1.00	23.91
7957	C	LEU	B	241	12.955	31.226	-8.384	1.00	22.17
7958	O	LEU	B	241	11.759	31.219	-8.613	1.00	22.86
7959	N	ASP	B	242	13.487	31.928	-7.401	1.00	22.89
7961	CA	ASP	B	242	12.680	32.816	-6.597	1.00	23.68
7963	CB	ASP	B	242	13.538	33.476	-5.526	1.00	24.26
7966	CG	ASP	B	242	12.782	33.732	-4.261	1.00	26.59
7967	OD1	ASP	B	242	12.339	34.885	-4.081	1.00	29.09
7968	OD2	ASP	B	242	12.586	32.842	-3.395	1.00	30.35
7969	C	ASP	B	242	12.018	33.889	-7.468	1.00	24.03
7970	O	ASP	B	242	10.872	34.264	-7.225	1.00	23.75
7971	N	VAL	B	243	12.722	34.380	-8.478	1.00	24.22
7973	CA	VAL	B	243	12.133	35.431	-9.334	1.00	25.09
7975	CB	BVAL	B	243	13.207	36.455	-9.871	0.35	24.92
7976	CB	AVAL	B	243	13.180	36.479	-9.849	0.65	25.18
7979	CG1	BVAL	B	243	14.454	35.767	-10.368	0.35	24.74
7980	CG1	AVAL	B	243	14.270	36.727	-8.817	0.65	24.27
7987	CG2	BVAL	B	243	12.633	37.361	-10.975	0.35	23.96
7988	CG2	AVAL	B	243	13.775	36.088	-11.166	0.65	25.87
7995	C	VAL	B	243	11.271	34.851	-10.474	1.00	25.74
7996	O	VAL	B	243	10.167	35.330	-10.688	1.00	25.89
7997	N	VAL	B	244	11.745	33.812	-11.160	1.00	26.96
7999	CA	VAL	B	244	11.065	33.282	-12.350	1.00	27.89
8001	CB	VAL	B	244	12.069	32.914	-13.472	1.00	28.15
8003	CG1	VAL	B	244	12.996	34.083	-13.769	1.00	29.48
8007	CG2	VAL	B	244	12.852	31.642	-13.143	1.00	28.31
8011	C	VAL	B	244	10.158	32.066	-12.136	1.00	28.41
8012	O	VAL	B	244	9.330	31.776	-12.983	1.00	28.51
8013	N	GLY	B	245	10.331	31.335	-11.038	1.00	29.07
8015	CA	GLY	B	245	9.583	30.107	-10.813	1.00	29.72
8018	C	GLY	B	245	8.131	30.378	-10.460	1.00	30.36
8019	O	GLY	B	245	7.793	31.482	-10.070	1.00	31.39
8020	N	ASP	B	246	7.276	29.376	-10.613	1.00	30.83
8022	CA	ASP	B	246	5.885	29.465	-10.194	1.00	31.66

FIGURE 3 ~~(Cont.)~~CZ

A	B	C	D	E	F	G	H	I	J
8024	CB	ASP	B	246	4.996	28.632	-11.128	1.00	32.32
8027	CG	ASP	B	246	3.527	29.006	-11.027	1.00	35.80
8028	OD1	ASP	B	246	2.981	29.516	-12.041	1.00	41.36
8029	OD2	ASP	B	246	2.818	28.820	-9.997	1.00	39.19
8030	C	ASP	B	246	5.782	28.894	-8.790	1.00	30.65
8031	O	ASP	B	246	6.321	27.842	-8.546	1.00	30.56
8032	N	THR	B	247	5.072	29.572	-7.892	1.00	29.92
8034	CA	THR	B	247	4.846	29.080	-6.533	1.00	29.76
8036	CB	THR	B	247	3.814	29.975	-5.811	1.00	29.87
8038	OG1	THR	B	247	4.378	31.272	-5.593	1.00	31.54
8040	CG2	THR	B	247	3.502	29.459	-4.399	1.00	30.40
8044	C	THR	B	247	4.401	27.611	-6.492	1.00	28.88
8045	O	THR	B	247	4.911	26.844	-5.685	1.00	28.30
8046	N	ALA	B	248	3.465	27.222	-7.358	1.00	28.23
8048	CA	ALA	B	248	2.932	25.852	-7.367	1.00	28.33
8050	CB	ALA	B	248	1.809	25.708	-8.391	1.00	28.17
8054	C	ALA	B	248	4.007	24.805	-7.644	1.00	28.26
8055	O	ALA	B	248	3.925	23.687	-7.143	1.00	28.69
8056	N	THR	B	249	4.985	25.172	-8.466	1.00	27.77
8058	CA	THR	B	249	6.091	24.292	-8.824	1.00	27.75
8060	CB	THR	B	249	6.638	24.726	-10.188	1.00	27.90
8062	OG1	THR	B	249	5.596	24.624	-11.164	1.00	30.21
8064	CG2	THR	B	249	7.706	23.767	-10.678	1.00	28.58
8068	C	THR	B	249	7.223	24.275	-7.773	1.00	26.85
8069	O	THR	B	249	7.671	23.202	-7.356	1.00	26.31
8070	N	LEU	B	250	7.654	25.463	-7.348	1.00	25.98
8072	CA	LEU	B	250	8.706	25.627	-6.328	1.00	25.67
8074	CB	LEU	B	250	8.994	27.116	-6.091	1.00	25.92
8077	CG	LEU	B	250	9.408	28.030	-7.239	1.00	27.52
8079	CD1	LEU	B	250	9.656	29.433	-6.691	1.00	27.93
8083	CD2	LEU	B	250	10.625	27.516	-7.954	1.00	28.70
8087	C	LEU	B	250	8.359	25.039	-4.965	1.00	24.61
8088	O	LEU	B	250	9.244	24.625	-4.217	1.00	22.99
8089	N	GLY	B	251	7.077	25.078	-4.612	1.00	23.96
8091	CA	GLY	B	251	6.636	24.759	-3.265	1.00	23.66
8094	C	GLY	B	251	6.808	25.892	-2.263	1.00	23.66
8095	O	GLY	B	251	6.449	25.748	-1.105	1.00	23.25
8096	N	LYS	B	252	7.310	27.036	-2.721	1.00	23.45
8098	CA	LYS	B	252	7.499	28.207	-1.881	1.00	23.55
8100	CB	LYS	B	252	8.913	28.217	-1.262	1.00	23.19
8103	CG	LYS	B	252	10.065	28.100	-2.279	1.00	22.81
8106	CD	LYS	B	252	11.443	27.892	-1.587	1.00	21.30
8109	CE	LYS	B	252	12.575	28.125	-2.537	1.00	19.95
8112	NZ	LYS	B	252	13.876	27.549	-2.087	1.00	18.06
8116	C	LYS	B	252	7.248	29.466	-2.729	1.00	24.42
8117	O	LYS	B	252	7.280	29.414	-3.961	1.00	24.38
8118	N	ARG	B	253	7.024	30.592	-2.066	1.00	25.44
8120	CA	ARG	B	253	6.534	31.795	-2.744	1.00	26.73
8122	CB	ARG	B	253	6.006	32.830	-1.737	1.00	27.67
8125	CG	ARG	B	253	4.510	33.101	-1.907	1.00	31.24
8128	CD	ARG	B	253	3.825	33.710	-0.700	1.00	35.52
8131	NE	ARG	B	253	3.150	32.704	0.116	1.00	37.39

FIGURE 3 ~~(Cont.)~~<u>DA</u>

A	B	C	D	E	F	G	H	I	J
8133	CZ	ARG	B	253	2.036	32.056	-0.235	1.00	39.88
8134	NH1	ARG	B	253	1.451	32.263	-1.417	1.00	41.43
8137	NH2	ARG	B	253	1.518	31.167	0.605	1.00	41.57
8140	C	ARG	B	253	7.550	32.432	-3.685	1.00	25.93
8141	O	ARG	B	253	8.642	32.852	-3.283	1.00	25.79
8142	N	GLN	B	254	7.176	32.480	-4.955	1.00	25.68
8144	CA	GLN	B	254	7.848	33.323	-5.931	1.00	25.41
8146	CB	GLN	B	254	7.076	33.337	-7.255	1.00	25.85
8149	CG	BGLN	B	254	7.707	34.187	-8.363	0.35	25.46
8150	CG	AGLN	B	254	7.696	34.266	-8.323	0.65	26.52
8155	CD	BGLN	B	254	7.388	35.665	-8.261	0.35	25.75
8156	CD	AGLN	B	254	6.858	34.376	-9.595	0.65	29.40
8157	OE1	BGLN	B	254	8.227	36.501	-8.593	0.35	26.04
8158	OE1	AGLN	B	254	7.335	34.901	-10.609	0.65	30.77
8159	NE2	BGLN	B	254	6.180	35.993	-7.809	0.35	25.98
8160	NE2	AGLN	B	254	5.622	33.888	-9.547	0.65	29.10
8165	C	GLN	B	254	7.900	34.730	-5.369	1.00	24.67
8166	O	GLN	B	254	6.942	35.184	-4.755	1.00	24.03
8167	N	GLY	B	255	9.023	35.413	-5.565	1.00	24.23
8169	CA	GLY	B	255	9.107	36.829	-5.264	1.00	24.15
8172	C	GLY	B	255	9.417	37.151	-3.816	1.00	24.34
8173	O	GLY	B	255	9.464	38.307	-3.465	1.00	24.07
8174	N	ALA	B	256	9.656	36.142	-2.983	1.00	24.66
8176	CA	ALA	B	256	9.909	36.359	-1.559	1.00	25.08
8178	CB	ALA	B	256	9.978	35.024	-0.833	1.00	24.93
8182	C	ALA	B	256	11.179	37.180	-1.288	1.00	25.56
8183	O	ALA	B	256	11.213	37.979	-0.353	1.00	26.42
8184	N	ASP	B	257	12.210	37.000	-2.105	1.00	25.88
8186	CA	ASP	B	257	13.466	37.739	-1.932	1.00	26.25
8188	CB	ASP	B	257	14.564	37.191	-2.848	1.00	26.11
8191	CG	ASP	B	257	15.025	35.791	-2.463	1.00	26.45
8192	OD1	ASP	B	257	14.815	35.353	-1.299	1.00	26.12
8193	OD2	ASP	B	257	15.602	35.054	-3.292	1.00	25.40
8194	C	ASP	B	257	13.286	39.221	-2.241	1.00	27.05
8195	O	ASP	B	257	13.823	40.074	-1.549	1.00	26.45
8196	N	GLN	B	258	12.545	39.520	-3.304	1.00	28.65
8198	CA	GLN	B	258	12.278	40.908	-3.691	1.00	29.67
8200	CB	BGLN	B	258	11.590	40.972	-5.061	0.35	29.64
8201	CB	AGLN	B	258	11.557	40.939	-5.046	0.65	30.10
8206	CG	BGLN	B	258	12.546	40.710	-6.226	0.35	29.64
8207	CG	AGLN	B	258	11.357	42.333	-5.625	0.65	31.67
8212	CD	BGLN	B	258	11.961	41.060	-7.589	0.35	29.88
8213	CD	AGLN	B	258	9.896	42.666	-5.883	0.65	33.37
8214	OE1	BGLN	B	258	12.242	40.380	-8.581	0.35	29.18
8215	OE1	AGLN	B	258	9.502	42.893	-7.025	0.65	34.64
8216	NE2	BGLN	B	258	11.163	42.126	-7.646	0.35	29.79
8217	NE2	AGLN	B	258	9.094	42.705	-4.820	0.65	34.91
8222	C	GLN	B	258	11.455	41.638	-2.614	1.00	29.97
8223	O	GLN	B	258	11.755	42.780	-2.274	1.00	29.34
8224	N	GLN	B	259	10.439	40.957	-2.080	1.00	30.70
8226	CA	GLN	B	259	9.658	41.427	-0.922	1.00	31.61
8228	CB	GLN	B	259	8.769	40.285	-0.410	1.00	32.41

FIGURE 3 ~~(Cont.)~~DB

A	B	C	D	E	F	G	H	I	J
8231	CG	GLN	B	259	7.466	40.703	0.244	1.00	35.31
8234	CD	GLN	B	259	6.317	40.769	-0.744	1.00	39.68
8235	OE1	GLN	B	259	5.925	41.861	-1.174	1.00	43.25
8236	NE2	GLN	B	259	5.780	39.605	-1.119	1.00	42.40
8239	C	GLN	B	259	10.546	41.934	0.242	1.00	31.29
8240	O	GLN	B	259	10.321	43.032	0.776	1.00	31.47
8241	N	LEU	B	260	11.552	41.135	0.612	1.00	30.18
8243	CA	LEU	B	260	12.421	41.420	1.761	1.00	29.88
8245	CB	LEU	B	260	12.851	40.109	2.446	1.00	29.79
8248	CG	LEU	B	260	11.792	39.268	3.160	1.00	30.18
8250	CD1	LEU	B	260	12.453	38.363	4.192	1.00	29.62
8254	CD2	LEU	B	260	10.742	40.140	3.817	1.00	31.47
8258	C	LEU	B	260	13.681	42.207	1.413	1.00	28.94
8259	O	LEU	B	260	14.431	42.593	2.307	1.00	29.69
8260	N	GLY	B	261	13.921	42.429	0.128	1.00	27.95
8262	CA	GLY	B	261	15.133	43.084	-0.333	1.00	26.93
8265	C	GLY	B	261	16.398	42.279	-0.094	1.00	25.88
8266	O	GLY	B	261	17.436	42.845	0.261	1.00	25.61
8267	N	LYS	B	262	16.325	40.959	-0.277	1.00	24.82
8269	CA	LYS	B	262	17.501	40.115	-0.136	1.00	23.75
8271	CB	LYS	B	262	17.153	38.627	-0.295	1.00	23.56
8274	CG	LYS	B	262	16.230	38.069	0.762	1.00	23.25
8277	CD	LYS	B	262	16.916	37.862	2.096	1.00	21.56
8280	CE	LYS	B	262	15.901	37.433	3.158	1.00	23.14
8283	NZ	LYS	B	262	16.536	37.070	4.482	1.00	21.85
8287	C	LYS	B	262	18.515	40.497	-1.195	1.00	23.58
8288	O	LYS	B	262	18.145	40.845	-2.337	1.00	23.29
8289	N	SER	B	263	19.785	40.474	-0.803	1.00	22.82
8291	CA	SER	B	263	20.885	40.514	-1.746	1.00	22.51
8293	CB	SER	B	263	22.206	40.785	-1.035	1.00	22.93
8296	OG	SER	B	263	22.263	42.141	-0.613	1.00	23.10
8298	C	SER	B	263	20.934	39.170	-2.452	1.00	22.79
8299	O	SER	B	263	21.051	38.122	-1.784	1.00	22.61
8300	N	THR	B	264	20.786	39.194	-3.782	1.00	21.90
8302	CA	THR	B	264	20.764	37.973	-4.593	1.00	22.01
8304	CB	THR	B	264	19.304	37.496	-4.909	1.00	22.17
8306	OG1	THR	B	264	18.667	38.392	-5.827	1.00	23.42
8308	CG2	THR	B	264	18.386	37.525	-3.707	1.00	21.68
8312	C	THR	B	264	21.499	38.175	-5.908	1.00	21.99
8313	O	THR	B	264	21.731	39.306	-6.354	1.00	21.16
8314	N	TYR	B	265	21.841	37.066	-6.553	1.00	21.84
8316	CA	TYR	B	265	22.470	37.134	-7.864	1.00	22.04
8318	CB	TYR	B	265	22.959	35.754	-8.319	1.00	21.34
8321	CG	TYR	B	265	24.340	35.435	-7.803	1.00	20.33
8322	CD1	TYR	B	265	25.430	35.422	-8.654	1.00	20.38
8324	CE1	TYR	B	265	26.686	35.129	-8.197	1.00	20.95
8326	CZ	TYR	B	265	26.877	34.859	-6.866	1.00	20.10
8327	OH	TYR	B	265	28.142	34.576	-6.417	1.00	24.40
8329	CE2	TYR	B	265	25.818	34.876	-5.989	1.00	19.89
8331	CD2	TYR	B	265	24.561	35.161	-6.455	1.00	18.52
8333	C	TYR	B	265	21.588	37.816	-8.933	1.00	22.40
8334	O	TYR	B	265	22.075	38.711	-9.612	1.00	22.20

FIGURE 3 (Cont.)DC

A	B	C	D	E	F	G	H	I	J
8335	N	PRO	B	266	20.328	37.413	-9.102	1.00	22.68
8336	CA	PRO	B	266	19.448	38.083	-10.073	1.00	23.28
8338	CB	PRO	B	266	18.131	37.309	-9.984	1.00	23.44
8341	CG	PRO	B	266	18.438	36.064	-9.253	1.00	23.26
8344	CD	PRO	B	266	19.635	36.319	-8.412	1.00	23.08
8347	C	PRO	B	266	19.193	39.550	-9.744	1.00	23.45
8348	O	PRO	B	266	19.084	40.350	-10.668	1.00	23.18
8349	N	ALA	B	267	19.099	39.890	-8.460	1.00	23.47
8351	CA	ALA	B	267	18.821	41.268	-8.062	1.00	23.58
8353	CB	ALA	B	267	18.569	41.386	-6.560	1.00	23.84
8357	C	ALA	B	267	19.962	42.155	-8.483	1.00	23.82
8358	O	ALA	B	267	19.742	43.216	-9.062	1.00	24.38
8359	N	LEU	B	268	21.184	41.692	-8.247	1.00	23.53
8361	CA	LEU	B	268	22.375	42.447	-8.586	1.00	23.59
8363	CB	LEU	B	268	23.566	41.908	-7.798	1.00	23.51
8366	CG	LEU	B	268	24.934	42.511	-8.113	1.00	23.92
8368	CD1	LEU	B	268	24.947	44.021	-7.830	1.00	24.92
8372	CD2	LEU	B	268	26.012	41.800	-7.318	1.00	24.12
8376	C	LEU	B	268	22.704	42.437	-10.082	1.00	23.25
8377	O	LEU	B	268	22.964	43.479	-10.664	1.00	23.31
8378	N	LEU	B	269	22.693	41.253	-10.683	1.00	22.76
8380	CA	LEU	B	269	23.281	41.018	-11.995	1.00	22.56
8382	CB	LEU	B	269	24.093	39.726	-11.983	1.00	22.53
8385	CG	LEU	B	269	25.314	39.686	-11.062	1.00	24.16
8387	CD1	LEU	B	269	25.881	38.277	-11.022	1.00	25.08
8391	CD2	LEU	B	269	26.394	40.674	-11.518	1.00	25.88
8395	C	LEU	B	269	22.237	40.925	-13.089	1.00	21.93
8396	O	LEU	B	269	22.567	40.925	-14.273	1.00	21.98
8397	N	GLY	B	270	20.981	40.880	-12.696	1.00	21.10
8399	CA	GLY	B	270	19.925	40.537	-13.619	1.00	21.48
8402	C	GLY	B	270	19.923	39.035	-13.860	1.00	21.79
8403	O	GLY	B	270	20.883	38.320	-13.530	1.00	20.41
8404	N	LEU	B	271	18.831	38.570	-14.445	1.00	22.27
8406	CA	LEU	B	271	18.587	37.145	-14.645	1.00	23.11
8408	CB	LEU	B	271	17.169	36.923	-15.161	1.00	23.57
8411	CG	LEU	B	271	16.145	36.966	-14.051	1.00	23.96
8413	CD1	LEU	B	271	14.712	36.988	-14.638	1.00	25.68
8417	CD2	LEU	B	271	16.375	35.748	-13.152	1.00	24.82
8421	C	LEU	B	271	19.554	36.493	-15.601	1.00	23.62
8422	O	LEU	B	271	19.999	35.393	-15.348	1.00	22.96
8423	N	GLU	B	272	19.885	37.158	-16.704	1.00	24.28
8425	CA	GLU	B	272	20.703	36.498	-17.715	1.00	25.35
8427	CB	GLU	B	272	20.712	37.237	-19.049	1.00	26.22
8430	CG	GLU	B	272	21.247	36.373	-20.184	1.00	30.72
8433	CD	GLU	B	272	20.177	35.523	-20.858	1.00	36.13
8434	OE1	GLU	B	272	19.801	35.857	-22.020	1.00	40.61
8435	OE2	GLU	B	272	19.725	34.513	-20.244	1.00	38.13
8436	C	GLU	B	272	22.116	36.293	-17.220	1.00	24.46
8437	O	GLU	B	272	22.658	35.215	-17.405	1.00	23.99
8438	N	GLN	B	273	22.707	37.305	-16.582	1.00	23.54
8440	CA	GLN	B	273	24.052	37.148	-16.019	1.00	23.89
8442	CB	GLN	B	273	24.640	38.488	-15.569	1.00	23.95

FIGURE 3 ~~(Cont.)~~DD

A	B	C	D	E	F	G	H	I	J
8445	CG	GLN	B	273	25.057	39.407	-16.701	1.00	26.62
8448	CD	GLN	B	273	25.436	40.804	-16.197	1.00	29.62
8449	OE1	GLN	B	273	26.041	40.939	-15.140	1.00	29.56
8450	NE2	GLN	B	273	25.046	41.834	-16.941	1.00	32.63
8453	C	GLN	B	273	24.042	36.157	-14.848	1.00	23.16
8454	O	GLN	B	273	24.994	35.428	-14.656	1.00	23.94
8455	N	ALA	B	274	22.968	36.130	-14.071	1.00	22.86
8457	CA	ALA	B	274	22.852	35.161	-12.985	1.00	22.78
8459	CB	ALA	B	274	21.591	35.413	-12.169	1.00	22.56
8463	C	ALA	B	274	22.848	33.738	-13.565	1.00	22.60
8464	O	ALA	B	274	23.542	32.873	-13.071	1.00	22.64
8465	N	ARG	B	275	22.085	33.520	-14.632	1.00	22.89
8467	CA	ARG	B	275	22.048	32.213	-15.299	1.00	23.30
8469	CB	ARG	B	275	21.012	32.205	-16.431	1.00	23.67
8472	CG	ARG	B	275	19.594	32.090	-15.944	1.00	25.28
8475	CD	ARG	B	275	18.542	32.199	-17.031	1.00	27.92
8478	NE	ARG	B	275	17.209	31.888	-16.503	1.00	30.36
8480	CZ	ARG	B	275	16.104	32.616	-16.697	1.00	32.35
8481	NH1	ARG	B	275	16.121	33.727	-17.423	1.00	31.95
8484	NH2	ARG	B	275	14.954	32.217	-16.160	1.00	34.03
8487	C	ARG	B	275	23.424	31.827	-15.854	1.00	23.20
8488	O	ARG	B	275	23.843	30.669	-15.783	1.00	22.27
8489	N	LYS	B	276	24.111	32.807	-16.421	1.00	23.01
8491	CA	LYS	B	276	25.418	32.595	-16.998	1.00	22.90
8493	CB	LYS	B	276	25.870	33.833	-17.774	1.00	23.16
8496	CG	LYS	B	276	27.307	33.794	-18.251	1.00	24.89
8499	CD	LYS	B	276	27.542	32.619	-19.190	1.00	28.29
8502	CE	LYS	B	276	28.672	32.892	-20.166	1.00	29.58
8505	NZ	LYS	B	276	29.948	33.113	-19.451	1.00	30.99
8509	C	LYS	B	276	26.422	32.253	-15.893	1.00	22.40
8510	O	LYS	B	276	27.270	31.400	-16.086	1.00	22.05
8511	N	LYS	B	277	26.312	32.901	-14.742	1.00	21.92
8513	CA	LYS	B	277	27.191	32.604	-13.612	1.00	22.26
8515	CB	LYS	B	277	26.959	33.566	-12.444	1.00	22.86
8518	CG	LYS	B	277	27.325	35.029	-12.759	1.00	26.57
8521	CD	LYS	B	277	28.574	35.530	-12.019	1.00	30.08
8524	CE	LYS	B	277	29.067	36.885	-12.583	1.00	31.95
8527	NZ	LYS	B	277	30.540	37.060	-12.449	1.00	33.10
8531	C	LYS	B	277	26.982	31.151	-13.175	1.00	21.47
8532	O	LYS	B	277	27.939	30.422	-12.944	1.00	21.43
8533	N	ALA	B	278	25.725	30.729	-13.101	1.00	20.57
8535	CA	ALA	B	278	25.408	29.366	-12.697	1.00	20.64
8537	CB	ALA	B	278	23.881	29.171	-12.552	1.00	20.42
8541	C	ALA	B	278	25.990	28.377	-13.699	1.00	20.27
8542	O	ALA	B	278	26.607	27.383	-13.306	1.00	19.24
8543	N	ARG	B	279	25.819	28.639	-14.990	1.00	20.74
8545	CA	ARG	B	279	26.307	27.695	-15.997	1.00	21.12
8547	CB	ARG	B	279	25.765	28.003	-17.392	1.00	21.76
8550	CG	ARG	B	279	26.088	26.897	-18.402	1.00	22.89
8553	CD	ARG	B	279	25.654	27.222	-19.814	1.00	25.89
8556	NE	ARG	B	279	26.498	28.272	-20.382	1.00	26.63
8558	CZ	ARG	B	279	26.296	28.833	-21.562	1.00	26.13

FIGURE 3 ~~(Cont.)~~DE

A	B	C	D	E	F	G	H	I	J
8559	NH1	ARG	B	279	25.253	28.490	-22.311	1.00	24.20
8562	NH2	ARG	B	279	27.138	29.760	-21.981	1.00	25.45
8565	C	ARG	B	279	27.831	27.650	-16.001	1.00	21.30
8566	O	ARG	B	279	28.416	26.590	-16.177	1.00	21.07
8567	N	ASP	B	280	28.461	28.795	-15.766	1.00	21.40
8569	CA	ASP	B	280	29.915	28.874	-15.595	1.00	21.87
8571	CB	ASP	B	280	30.335	30.327	-15.313	1.00	22.54
8574	CG	ASP	B	280	30.370	31.200	-16.579	1.00	25.24
8575	OD1	ASP	B	280	30.630	32.424	-16.457	1.00	28.05
8576	OD2	ASP	B	280	30.138	30.759	-17.724	1.00	26.91
8577	C	ASP	B	280	30.401	27.958	-14.456	1.00	21.04
8578	O	ASP	B	280	31.440	27.297	-14.562	1.00	20.76
8579	N	LEU	B	281	29.633	27.922	-13.372	1.00	20.21
8581	CA	LEU	B	281	29.994	27.151	-12.188	1.00	19.69
8583	CB	LEU	B	281	29.141	27.569	-10.992	1.00	19.82
8586	CG	LEU	B	281	29.530	28.953	-10.452	1.00	18.53
8588	CD1	LEU	B	281	28.423	29.532	-9.589	1.00	19.63
8592	CD2	LEU	B	281	30.812	28.869	-9.646	1.00	19.99
8596	C	LEU	B	281	29.838	25.670	-12.468	1.00	19.73
8597	O	LEU	B	281	30.671	24.889	-12.094	1.00	20.05
8598	N	ILE	B	282	28.774	25.295	-13.150	1.00	20.33
8600	CA	ILE	B	282	28.597	23.906	-13.555	1.00	21.14
8602	CB	ILE	B	282	27.190	23.672	-14.076	1.00	21.02
8604	CG1	ILE	B	282	26.178	23.925	-12.949	1.00	22.56
8607	CD1	ILE	B	282	26.532	23.265	-11.610	1.00	22.71
8611	CG2	ILE	B	282	27.041	22.244	-14.624	1.00	21.66
8615	C	ILE	B	282	29.659	23.477	-14.566	1.00	21.32
8616	O	ILE	B	282	30.149	22.359	-14.488	1.00	21.92
8617	N	ASP	B	283	30.032	24.358	-15.487	1.00	21.87
8619	CA	ASP	B	283	31.112	24.056	-16.430	1.00	22.32
8621	CB	ASP	B	283	31.436	25.261	-17.330	1.00	22.60
8624	CG	ASP	B	283	30.410	25.503	-18.417	1.00	23.70
8625	OD1	ASP	B	283	30.445	26.623	-18.989	1.00	26.27
8626	OD2	ASP	B	283	29.548	24.676	-18.786	1.00	22.23
8627	C	ASP	B	283	32.369	23.705	-15.624	1.00	22.25
8628	O	ASP	B	283	33.066	22.756	-15.928	1.00	21.47
8629	N	ASP	B	284	32.636	24.490	-14.588	1.00	22.34
8631	CA	ASP	B	284	33.793	24.291	-13.731	1.00	23.23
8633	CB	ASP	B	284	33.980	25.509	-12.820	1.00	23.34
8636	CG	ASP	B	284	35.161	25.368	-11.918	1.00	26.31
8637	OD1	ASP	B	284	36.305	25.530	-12.420	1.00	28.34
8638	OD2	ASP	B	284	35.037	25.088	-10.697	1.00	28.06
8639	C	ASP	B	284	33.670	22.986	-12.925	1.00	22.69
8640	O	ASP	B	284	34.641	22.234	-12.816	1.00	22.49
8641	N	ALA	B	285	32.474	22.703	-12.405	1.00	22.19
8643	CA	ALA	B	285	32.204	21.431	-11.725	1.00	22.57
8645	CB	ALA	B	285	30.752	21.361	-11.263	1.00	22.03
8649	C	ALA	B	285	32.524	20.233	-12.631	1.00	22.99
8650	O	ALA	B	285	33.151	19.270	-12.190	1.00	22.66
8651	N	ARG	B	286	32.115	20.321	-13.895	1.00	23.78
8653	CA	ARG	B	286	32.394	19.283	-14.883	1.00	25.16
8655	CB	ARG	B	286	31.628	19.550	-16.180	1.00	25.91

FIGURE 3 ~~(Cont.)~~DF

A	B	C	D	E	F	G	H	I	J
8658	CG	ARG	B	286	30.138	19.170	-16.097	1.00	28.32
8661	CD B	ARG	B	286	29.468	18.992	-17.466	0.35	29.52
8662	CD A	ARG	B	286	29.453	19.007	-17.451	0.65	30.92
8667	NE B	ARG	B	286	29.262	20.264	-18.163	0.35	29.83
8668	NE A	ARG	B	286	28.271	18.146	-17.365	0.65	31.71
8671	CZ B	ARG	B	286	28.839	20.386	-19.423	0.35	30.53
8672	CZ A	ARG	B	286	28.231	16.856	-17.684	0.65	33.32
8673	NH1B	ARG	B	286	28.567	19.313	-20.165	0.35	30.23
8674	NH1A	ARG	B	286	29.309	16.209	-18.125	0.65	33.00
8679	NH2B	ARG	B	286	28.688	21.596	-19.951	0.35	30.87
8680	NH2A	ARG	B	286	27.089	16.195	-17.563	0.65	33.96
8685	C	ARG	B	286	33.894	19.108	-15.170	1.00	25.22
8686	O	ARG	B	286	34.349	17.988	-15.388	1.00	24.81
8687	N	GLN	B	287	34.651	20.204	-15.171	1.00	25.23
8689	CA	GLN	B	287	36.100	20.116	-15.322	1.00	25.93
8691	CB	GLN	B	287	36.756	21.497	-15.472	1.00	26.28
8694	CG	GLN	B	287	36.425	22.206	-16.775	1.00	29.31
8697	CD	GLN	B	287	37.009	21.533	-18.012	1.00	32.74
8698	OE1	GLN	B	287	38.047	20.880	-17.945	1.00	35.76
8699	NE2	GLN	B	287	36.340	21.706	-19.144	1.00	35.59
8702	C	GLN	B	287	36.706	19.364	-14.131	1.00	25.31
8703	O	GLN	B	287	37.565	18.521	-14.333	1.00	24.00
8704	N	SER	B	288	36.241	19.658	-12.905	1.00	25.12
8706	CA	SER	B	288	36.665	18.911	-11.720	1.00	25.39
8708	CB	SER	B	288	36.105	19.510	-10.414	1.00	25.38
8711	OG	SER	B	288	36.557	20.834	-10.215	1.00	24.82
8713	C	SER	B	288	36.289	17.433	-11.820	1.00	25.78
8714	O	SER	B	288	37.077	16.569	-11.459	1.00	25.49
8715	N	LEU	B	289	35.098	17.125	-12.321	1.00	26.38
8717	CA	LEU	B	289	34.709	15.726	-12.441	1.00	27.10
8719	CB	LEU	B	289	33.237	15.580	-12.838	1.00	26.93
8722	CG	LEU	B	289	32.258	15.977	-11.729	1.00	25.30
8724	CD1	LEU	B	289	30.821	15.804	-12.200	1.00	25.85
8728	CD2	LEU	B	289	32.524	15.189	-10.431	1.00	25.23
8732	C	LEU	B	289	35.635	14.995	-13.425	1.00	28.16
8733	O	LEU	B	289	35.998	13.854	-13.186	1.00	28.16
8734	N	LYS	B	290	36.053	15.677	-14.487	1.00	29.02
8736	CA	LYS	B	290	36.961	15.096	-15.481	1.00	30.79
8738	CB	LYS	B	290	37.313	16.118	-16.587	1.00	30.97
8741	CG	LYS	B	290	36.966	15.687	-18.011	1.00	33.97
8744	CD	LYS	B	290	36.614	16.900	-18.921	1.00	36.64
8747	CE	LYS	B	290	35.099	17.019	-19.182	1.00	37.79
8750	NZ	LYS	B	290	34.637	18.445	-19.343	1.00	38.84
8754	C	LYS	B	290	38.244	14.611	-14.809	1.00	31.28
8755	O	LYS	B	290	38.750	13.544	-15.141	1.00	31.44
8756	N	GLN	B	291	38.759	15.401	-13.869	1.00	32.13
8758	CA	GLN	B	291	39.978	15.054	-13.152	1.00	33.58
8760	CB	GLN	B	291	40.470	16.251	-12.326	1.00	33.80
8763	CG	GLN	B	291	40.818	17.493	-13.167	1.00	35.12
8766	CD	GLN	B	291	40.846	18.775	-12.353	1.00	36.83
8767	OE1	GLN	B	291	41.175	18.756	-11.168	1.00	36.95
8768	NE2	GLN	B	291	40.495	19.893	-12.985	1.00	38.40

FIGURE 3 ~~(Cont.)~~<u>DG</u>

A	B	C	D	E	F	G	H	I	J
8771	C	GLN	B	291	39.800	13.810	-12.265	1.00	34.42
8772	O	GLN	B	291	40.764	13.098	-12.013	1.00	34.62
8773	N	LEU	B	292	38.577	13.568	-11.784	1.00	35.42
8775	CA	LEU	B	292	38.248	12.364	-10.999	1.00	36.35
8777	CB	LEU	B	292	36.931	12.542	-10.251	1.00	36.39
8780	CG	LEU	B	292	36.924	13.515	-9.082	1.00	36.49
8782	CD1	LEU	B	292	35.562	13.491	-8.411	1.00	36.85
8786	CD2	LEU	B	292	38.023	13.153	-8.101	1.00	36.84
8790	C	LEU	B	292	38.141	11.088	-11.820	1.00	37.54
8791	O	LEU	B	292	38.519	10.015	-11.352	1.00	37.33
8792	N	ALA	B	293	37.598	11.193	-13.028	1.00	38.95
8794	CA	ALA	B	293	37.635	10.088	-13.974	1.00	40.14
8796	CB	ALA	B	293	36.587	10.291	-15.078	1.00	40.36
8800	C	ALA	B	293	39.045	9.950	-14.565	1.00	40.76
8801	O	ALA	B	293	39.206	9.462	-15.677	1.00	41.94
8802	N	GLU	B	294	40.045	10.442	-13.834	1.00	41.22
8804	CA	GLU	B	294	41.456	10.118	-14.039	1.00	41.53
8806	CB	GLU	B	294	42.240	11.402	-14.318	1.00	41.94
8809	CG	GLU	B	294	43.620	11.186	-14.911	1.00	44.01
8812	CD	GLU	B	294	44.144	12.428	-15.604	1.00	45.96
8813	OE1	GLU	B	294	44.166	13.499	-14.953	1.00	48.06
8814	OE2	GLU	B	294	44.528	12.332	-16.794	1.00	47.73
8815	C	GLU	B	294	42.047	9.414	-12.808	1.00	40.89
8816	O	GLU	B	294	43.185	8.941	-12.846	1.00	41.57
8817	N	GLN	B	295	41.295	9.399	-11.705	1.00	39.90
8819	CA	GLN	B	295	41.549	8.516	-10.565	1.00	38.66
8821	CB	GLN	B	295	41.248	9.243	-9.243	1.00	38.65
8824	CG	GLN	B	295	41.958	10.592	-9.083	1.00	38.47
8827	CD	GLN	B	295	41.556	11.354	-7.816	1.00	37.66
8828	OE1	GLN	B	295	41.179	10.751	-6.807	1.00	36.11
8829	NE2	GLN	B	295	41.658	12.686	-7.867	1.00	36.75
8832	C	GLN	B	295	40.681	7.258	-10.689	1.00	37.75
8833	O	GLN	B	295	40.432	6.560	-9.698	1.00	37.50
8834	N	SER	B	296	40.220	6.995	-11.914	1.00	36.44
8836	CA	SER	B	296	39.373	5.852	-12.261	1.00	35.92
8838	CB	SER	B	296	40.117	4.541	-12.022	1.00	36.22
8841	OG	SER	B	296	39.666	3.572	-12.955	1.00	38.05
8843	C	SER	B	296	38.003	5.810	-11.566	1.00	34.56
8844	O	SER	B	296	37.551	4.753	-11.143	1.00	34.47
8845	N	LEU	B	297	37.330	6.952	-11.485	1.00	32.72
8847	CA	LEU	B	297	36.060	7.022	-10.773	1.00	31.10
8849	CB	LEU	B	297	36.114	8.107	-9.699	1.00	30.86
8852	CG	LEU	B	297	37.166	7.891	-8.611	1.00	30.39
8854	CD1	LEU	B	297	37.381	9.150	-7.786	1.00	30.04
8858	CD2	LEU	B	297	36.771	6.739	-7.721	1.00	30.69
8862	C	LEU	B	297	34.910	7.286	-11.724	1.00	30.21
8863	O	LEU	B	297	35.045	8.047	-12.684	1.00	29.81
8864	N	ASP	B	298	33.776	6.655	-11.425	1.00	28.91
8866	CA	ASP	B	298	32.541	6.834	-12.171	1.00	28.55
8868	CB	ASP	B	298	31.659	5.597	-12.005	1.00	28.67
8871	CG	ASP	B	298	30.377	5.661	-12.823	1.00	30.58
8872	OD1	ASP	B	298	30.141	6.682	-13.512	1.00	31.79

FIGURE 3 ~~(Cont.)~~<u>DH</u>

A	B	C	D	E	F	G	H	I	J
8873	OD2	ASP	B	298	29.534	4.729	-12.815	1.00	33.35
8874	C	ASP	B	298	31.830	8.086	-11.662	1.00	27.64
8875	O	ASP	B	298	31.132	8.050	-10.649	1.00	26.94
8876	N	THR	B	299	32.007	9.187	-12.390	1.00	26.96
8878	CA	THR	B	299	31.424	10.478	-12.020	1.00	26.33
8880	CB	THR	B	299	32.352	11.615	-12.471	1.00	26.05
8882	OG1	THR	B	299	32.571	11.538	-13.882	1.00	27.18
8884	CG2	THR	B	299	33.740	11.457	-11.879	1.00	26.15
8888	C	THR	B	299	30.006	10.704	-12.588	1.00	25.98
8889	O	THR	B	299	29.464	11.785	-12.453	1.00	25.98
8890	N	SER	B	300	29.392	9.682	-13.176	1.00	25.39
8892	CA	SER	B	300	28.130	9.855	-13.906	1.00	25.11
8894	CB	SER	B	300	27.672	8.535	-14.531	1.00	25.29
8897	OG	SER	B	300	27.346	7.581	-13.529	1.00	27.52
8899	C	SER	B	300	27.004	10.479	-13.077	1.00	24.18
8900	O	SER	B	300	26.340	11.391	-13.553	1.00	23.89
8901	N	ALA	B	301	26.788	10.001	-11.850	1.00	23.33
8903	CA	ALA	B	301	25.756	10.590	-10.983	1.00	22.98
8905	CB	ALA	B	301	25.555	9.776	-9.736	1.00	22.98
8909	C	ALA	B	301	26.051	12.044	-10.605	1.00	22.43
8910	O	ALA	B	301	25.138	12.850	-10.585	1.00	21.51
8911	N	LEU	B	302	27.321	12.361	-10.309	1.00	22.10
8913	CA	LEU	B	302	27.705	13.698	-9.887	1.00	21.91
8915	CB	LEU	B	302	29.102	13.715	-9.268	1.00	21.74
8918	CG	LEU	B	302	29.295	12.964	-7.951	1.00	22.89
8920	CD1	LEU	B	302	30.736	13.126	-7.523	1.00	23.47
8924	CD2	LEU	B	302	28.338	13.420	-6.858	1.00	23.02
8928	C	LEU	B	302	27.651	14.663	-11.058	1.00	22.32
8929	O	LEU	B	302	27.411	15.858	-10.863	1.00	21.59
8930	N	GLU	B	303	27.861	14.144	-12.270	1.00	22.83
8932	CA	GLU	B	303	27.716	14.933	-13.480	1.00	23.58
8934	CB	GLU	B	303	28.227	14.192	-14.720	1.00	24.19
8937	CG	GLU	B	303	29.708	13.867	-14.789	1.00	27.75
8940	CD	GLU	B	303	30.025	12.941	-15.962	1.00	31.36
8941	OE1	GLU	B	303	29.515	13.205	-17.070	1.00	34.68
8942	OE2	GLU	B	303	30.758	11.938	-15.784	1.00	33.57
8943	C	GLU	B	303	26.241	15.247	-13.705	1.00	23.21
8944	O	GLU	B	303	25.897	16.382	-14.000	1.00	23.30
8945	N	ALA	B	304	25.378	14.238	-13.592	1.00	22.93
8947	CA	ALA	B	304	23.954	14.418	-13.865	1.00	23.17
8949	CB	ALA	B	304	23.219	13.063	-13.846	1.00	23.72
8953	C	ALA	B	304	23.348	15.383	-12.844	1.00	22.99
8954	O	ALA	B	304	22.530	16.240	-13.186	1.00	22.84
8955	N	LEU	B	305	23.786	15.250	-11.596	1.00	22.47
8957	CA	LEU	B	305	23.331	16.111	-10.518	1.00	22.39
8959	CB	LEU	B	305	23.841	15.623	-9.166	1.00	22.42
8962	CG	LEU	B	305	23.319	16.420	-7.973	1.00	23.49
8964	CD1	LEU	B	305	21.813	16.473	-7.938	1.00	26.09
8968	CD2	LEU	B	305	23.835	15.859	-6.701	1.00	25.91
8972	C	LEU	B	305	23.766	17.540	-10.732	1.00	21.68
8973	O	LEU	B	305	22.993	18.452	-10.511	1.00	21.68
8974	N	ALA	B	306	25.002	17.742	-11.173	1.00	21.62

FIGURE 3 (Cont.)DI

A	B	C	D	E	F	G	H	I	J
8976	CA	ALA	B	306	25.507	19.094	-11.401	1.00	21.18
8978	CB	ALA	B	306	26.970	19.055	-11.829	1.00	20.99
8982	C	ALA	B	306	24.649	19.827	-12.437	1.00	21.29
8983	O	ALA	B	306	24.260	20.978	-12.221	1.00	20.84
8984	N	ASP	B	307	24.356	19.157	-13.557	1.00	21.52
8986	CA	ASP	B	307	23.462	19.700	-14.575	1.00	21.89
8988	CB	ASP	B	307	23.298	18.717	-15.749	1.00	22.19
8991	CG	ASP	B	307	24.484	18.721	-16.695	1.00	24.91
8992	OD1	ASP	B	307	25.217	19.734	-16.774	1.00	27.76
8993	OD2	ASP	B	307	24.754	17.744	-17.418	1.00	28.49
8994	C	ASP	B	307	22.091	19.989	-13.985	1.00	21.17
8995	O	ASP	B	307	21.517	21.065	-14.199	1.00	21.04
8996	N	TYR	B	308	21.566	19.037	-13.226	1.00	20.68
8998	CA	TYR	B	308	20.230	19.196	-12.667	1.00	21.00
9000	CB	TYR	B	308	19.804	17.946	-11.921	1.00	20.75
9003	CG	TYR	B	308	18.419	18.039	-11.344	1.00	21.19
9004	CD1	TYR	B	308	18.220	18.052	-9.966	1.00	20.91
9006	CE1	TYR	B	308	16.956	18.127	-9.432	1.00	21.89
9008	CZ	TYR	B	308	15.853	18.187	-10.268	1.00	24.30
9009	OH	TYR	B	308	14.587	18.254	-9.704	1.00	26.37
9011	CE2	TYR	B	308	16.020	18.192	-11.643	1.00	23.04
9013	CD2	TYR	B	308	17.299	18.112	-12.174	1.00	22.71
9015	C	TYR	B	308	20.145	20.397	-11.726	1.00	21.05
9016	O	TYR	B	308	19.109	21.018	-11.613	1.00	20.68
9017	N	ILE	B	309	21.239	20.713	-11.043	1.00	21.13
9019	CA	ILE	B	309	21.245	21.825	-10.102	1.00	21.51
9021	CB	ILE	B	309	22.635	21.881	-9.382	1.00	21.42
9023	CG1	ILE	B	309	22.663	20.817	-8.279	1.00	21.51
9026	CD1	ILE	B	309	24.007	20.664	-7.593	1.00	22.06
9030	CG2	ILE	B	309	22.891	23.256	-8.766	1.00	22.35
9034	C	ILE	B	309	20.874	23.159	-10.774	1.00	21.80
9035	O	ILE	B	309	20.237	24.017	-10.162	1.00	21.41
9036	N	ILE	B	310	21.245	23.328	-12.041	1.00	22.74
9038	CA	ILE	B	310	20.886	24.542	-12.765	1.00	23.55
9040	CB	ILE	B	310	22.148	25.209	-13.364	1.00	23.89
9042	CG1	ILE	B	310	22.714	24.400	-14.540	1.00	24.25
9045	CD1	ILE	B	310	23.776	25.141	-15.342	1.00	24.35
9049	CG2	ILE	B	310	23.190	25.406	-12.269	1.00	24.66
9053	C	ILE	B	310	19.799	24.344	-13.828	1.00	23.85
9054	O	ILE	B	310	19.400	25.315	-14.470	1.00	24.70
9055	N	GLN	B	311	19.319	23.110	-14.015	1.00	23.74
9057	CA	GLN	B	311	18.251	22.833	-14.990	1.00	23.91
9059	CB	GLN	B	311	18.584	21.602	-15.821	1.00	24.17
9062	CG	GLN	B	311	19.713	21.884	-16.815	1.00	26.77
9065	CD	GLN	B	311	20.172	20.670	-17.588	1.00	28.31
9066	OE1	GLN	B	311	21.115	20.760	-18.367	1.00	33.64
9067	NE2	GLN	B	311	19.520	19.540	-17.382	1.00	32.21
9070	C	GLN	B	311	16.887	22.687	-14.329	1.00	23.46
9071	O	GLN	B	311	15.857	22.873	-14.981	1.00	23.30
9072	N	ARG	B	312	16.889	22.369	-13.033	1.00	23.14
9074	CA	ARG	B	312	15.666	22.175	-12.249	1.00	22.83
9076	CB	ARG	B	312	16.010	21.784	-10.806	1.00	22.67

FIGURE 3 (Cont.)DJ

A	B	C	D	E	F	G	H	I	J
9079	CG	ARG	B	312	16.722	22.887	-10.002	1.00	21.91
9082	CD	ARG	B	312	17.584	22.348	-8.871	1.00	20.80
9085	NE	ARG	B	312	18.319	23.405	-8.180	1.00	19.32
9087	CZ	ARG	B	312	17.807	24.145	-7.212	1.00	19.88
9088	NH1	ARG	B	312	18.559	25.083	-6.640	1.00	20.86
9091	NH2	ARG	B	312	16.547	23.956	-6.806	1.00	18.83
9094	C	ARG	B	312	14.826	23.434	-12.199	1.00	23.29
9095	O	ARG	B	312	15.361	24.542	-12.222	1.00	22.52
9096	N	ASN	B	313	13.513	23.232	-12.116	1.00	24.23
9098	CA	ASN	B	313	12.519	24.294	-11.967	1.00	25.30
9100	CB	ASN	B	313	11.404	24.132	-13.023	1.00	25.73
9103	CG	ASN	B	313	10.586	22.855	-12.843	1.00	27.06
9104	OD1	ASN	B	313	10.893	22.015	-12.003	1.00	30.28
9105	ND2	ASN	B	313	9.526	22.712	-13.642	1.00	30.33
9108	C	ASN	B	313	11.922	24.303	-10.550	1.00	26.15
9109	O	ASN	B	313	10.931	24.991	-10.282	1.00	26.07
9110	N	LYS	B	314	12.523	23.510	-9.663	1.00	26.76
9112	CA	LYS	B	314	12.057	23.349	-8.295	1.00	27.55
9114	CB	LYS	B	314	10.997	22.245	-8.214	1.00	28.24
9117	CG	LYS	B	314	11.437	20.876	-8.748	1.00	30.42
9120	CD	LYS	B	314	10.388	19.777	-8.483	1.00	34.02
9123	CE	LYS	B	314	9.281	19.733	-9.557	1.00	35.81
9126	NZ	LYS	B	314	9.763	19.297	-10.914	1.00	37.55
9130	C	LYS	B	314	13.212	23.017	-7.370	1.00	27.53
9131	O	LYS	B	314	13.045	23.018	-6.148	1.00	27.94
9132	OXT	LYS	B	314	14.311	22.729	-7.848	1.00	26.55
9133	O9	ipp	X	900	59.879	67.784	6.844	1.00	22.62
9134	P7	ipp	X	900	60.281	67.030	8.078	1.00	20.44
9135	O8	ipp	X	900	61.128	65.793	7.905	1.00	20.16
9136	O10	ipp	X	900	58.921	66.747	8.923	1.00	20.32
9137	P11	ipp	X	900	58.096	65.364	9.039	1.00	20.72
9138	O13	ipp	X	900	58.271	64.667	7.712	1.00	21.48
9139	O12	ipp	X	900	58.760	64.598	10.167	1.00	20.42
9140	O14	ipp	X	900	56.677	65.719	9.388	1.00	19.87
9141	O6	ipp	X	900	61.085	68.067	9.000	1.00	23.40
9142	C5	ipp	X	900	60.446	69.278	9.396	1.00	22.55
9145	C4	ipp	X	900	61.386	70.077	10.277	1.00	23.87
9148	C2	ipp	X	900	62.729	70.303	9.627	1.00	24.00
9149	C3	ipp	X	900	62.847	70.872	8.237	1.00	23.48
9153	C1	ipp	X	900	63.818	70.021	10.311	1.00	24.77
9156	O12	ris	X	901	57.820	74.304	11.572	1.00	21.28
9157	P9	ris	X	901	58.623	73.691	10.433	1.00	21.35
9158	O11	ris	X	901	58.329	74.511	8.992	1.00	22.29
9160	O10	ris	X	901	58.206	72.094	10.263	1.00	22.10
9162	C8	ris	X	901	60.334	73.798	10.791	1.00	20.58
9163	O13	ris	X	901	61.051	73.167	9.710	1.00	21.47
9165	P14	ris	X	901	60.832	75.467	10.955	1.00	21.49
9166	O16	ris	X	901	60.487	76.175	9.664	1.00	20.67
9167	O15	ris	X	901	60.014	76.127	12.259	1.00	20.29
9169	O17	ris	X	901	62.473	75.654	11.235	1.00	16.79
9171	C7	ris	X	901	60.517	73.036	12.110	1.00	20.01
9174	C2	ris	X	901	61.916	72.843	12.658	1.00	20.04

FIGURE 3 (~~Cont.~~)DK

A	B	C	D	E	F	G	H	I	J
9175	C1	ris	X	901	62.030	72.693	14.038	1.00	22.23
9177	C6	ris	X	901	63.284	72.496	14.614	1.00	21.92
9179	C5	ris	X	901	64.396	72.454	13.790	1.00	21.90
9181	N4	ris	X	901	64.272	72.597	12.461	1.00	20.50
9182	C3	ris	X	901	63.073	72.787	11.887	1.00	20.38
9184	O9	ipp	X	902	16.064	23.295	-2.975	1.00	21.48
9185	P7	ipp	X	902	16.496	22.587	-1.731	1.00	20.32
9186	O8	ipp	X	902	17.402	21.368	-1.817	1.00	20.60
9187	O10	ipp	X	902	15.180	22.297	-0.852	1.00	19.29
9188	P11	ipp	X	902	14.357	20.933	-0.731	1.00	21.41
9189	O13	ipp	X	902	14.501	20.303	-2.099	1.00	21.14
9190	O12	ipp	X	902	15.018	20.139	0.361	1.00	19.56
9191	O14	ipp	X	902	12.943	21.318	-0.386	1.00	20.18
9192	O6	ipp	X	902	17.282	23.658	-0.828	1.00	21.57
9193	C5	ipp	X	902	16.665	24.901	-0.520	1.00	20.59
9196	C4	ipp	X	902	17.539	25.684	0.451	1.00	20.72
9199	C2	ipp	X	902	18.923	25.954	-0.086	1.00	20.12
9200	C3	ipp	X	902	19.094	26.613	-1.425	1.00	20.10
9204	C1	ipp	X	902	19.970	25.641	0.637	1.00	19.72
9207	O12	ris	X	903	13.949	29.944	1.653	1.00	18.96
9208	P9	ris	X	903	14.827	29.319	0.595	1.00	18.15
9209	O11	ris	X	903	14.564	30.066	-0.891	1.00	17.76
9211	O10	ris	X	903	14.479	27.699	0.371	1.00	17.12
9213	C8	ris	X	903	16.543	29.484	1.000	1.00	16.83
9214	O13	ris	X	903	17.268	28.905	-0.099	1.00	14.71
9216	P14	ris	X	903	17.105	31.143	1.147	1.00	16.07
9217	O16	ris	X	903	16.424	31.703	2.361	1.00	18.08
9218	O15	ris	X	903	18.754	31.239	1.421	1.00	20.15
9220	O17	ris	X	903	16.681	31.883	-0.303	1.00	17.24
9222	C7	ris	X	903	16.736	28.711	2.310	1.00	15.64
9225	C2	ris	X	903	18.144	28.461	2.843	1.00	17.89
9226	C1	ris	X	903	18.231	28.146	4.193	1.00	17.51
9228	C6	ris	X	903	19.477	27.908	4.776	1.00	17.87
9230	C5	ris	X	903	20.612	27.985	3.980	1.00	18.68
9232	N4	ris	X	903	20.535	28.281	2.665	1.00	18.45
9233	C3	ris	X	903	19.332	28.506	2.084	1.00	18.77
9235	MG	MG	X	904	15.574	31.310	-1.873	1.00	21.07
9236	MG	MG	X	905	17.080	32.751	3.968	1.00	17.94
9237	MG	MG	X	906	14.279	31.564	2.944	1.00	18.98
9238	MG	MG	X	907	58.027	75.928	12.811	1.00	21.97
9239	MG	MG	X	908	59.508	75.731	8.080	1.00	25.32
9240	MG	MG	X	909	60.807	77.116	13.792	1.00	19.86
9241	OW0	HOH	X	1	69.581	70.101	13.536	1.00	18.91
9244	OW0	HOH	X	2	62.678	62.339	10.204	1.00	15.42
9247	OW0	HOH	X	3	25.799	25.747	3.926	1.00	15.73
9250	OW0	HOH	X	4	59.333	62.010	10.213	1.00	18.17
9253	OW0	HOH	X	5	18.822	17.964	0.386	1.00	18.32
9256	OW0	HOH	X	6	13.596	24.842	-2.548	1.00	13.98
9259	OW0	HOH	X	7	60.443	70.120	5.487	1.00	20.05
9262	OW0	HOH	X	8	67.024	68.022	10.947	1.00	18.31
9265	OW0	HOH	X	9	75.891	66.532	13.529	1.00	16.24
9268	OW0	HOH	X	10	61.389	59.407	28.540	1.00	15.76

FIGURE 3 (Cont.)DL

A	B	C	D	E	F	G	H	I	J
9271	OW0	HOH	X	11	16.713	25.479	-4.403	1.00	16.69
9274	OW0	HOH	X	12	17.228	19.008	-1.948	1.00	17.97
9277	OW0	HOH	X	13	60.948	63.338	7.816	1.00	17.21
9280	OW0	HOH	X	14	12.537	21.690	6.873	1.00	20.29
9283	OW0	HOH	X	15	17.395	34.432	2.680	1.00	15.95
9286	OW0	HOH	X	16	22.715	24.983	3.509	1.00	21.00
9289	OW0	HOH	X	17	23.103	23.679	1.175	1.00	16.66
9292	OW0	HOH	X	18	60.488	77.235	6.934	1.00	16.27
9295	OW0	HOH	X	19	57.327	69.233	7.233	1.00	17.06
9298	OW0	HOH	X	20	15.505	17.649	0.655	1.00	17.89
9301	OW0	HOH	X	21	34.673	22.728	-9.839	1.00	22.21
9304	OW0	HOH	X	22	12.191	23.940	-0.324	1.00	14.99
9307	OW0	HOH	X	23	4.461	26.280	19.031	1.00	23.20
9310	OW0	HOH	X	24	72.420	88.509	2.009	1.00	28.92
9313	OW0	HOH	X	25	73.365	71.690	24.882	1.00	15.83
9316	OW0	HOH	X	26	9.311	27.134	10.014	1.00	16.86
9319	OW0	HOH	X	27	33.303	4.388	14.111	1.00	23.61
9322	OW0	HOH	X	28	9.972	29.039	2.416	1.00	19.40
9325	OW0	HOH	X	29	20.315	24.167	4.178	1.00	21.86
9328	OW0	HOH	X	30	23.161	10.579	20.659	1.00	23.73
9331	OW0	HOH	X	31	62.889	76.521	13.608	1.00	18.10
9334	OW0	HOH	X	32	14.368	17.510	4.944	1.00	24.43
9337	OW0	HOH	X	33	31.222	26.334	11.934	1.00	21.87
9340	OW0	HOH	X	34	17.123	34.428	-0.050	1.00	18.82
9343	OW0	HOH	X	35	65.244	84.346	-6.827	1.00	23.12
9346	OW0	HOH	X	36	53.273	71.292	19.938	1.00	20.38
9349	OW0	HOH	X	37	75.108	70.654	21.698	1.00	19.01
9352	OW0	HOH	X	38	61.370	78.383	15.450	1.00	24.45
9355	OW0	HOH	X	39	64.170	68.585	13.753	1.00	23.11
9358	OW0	HOH	X	40	15.187	3.524	-3.226	1.00	21.48
9361	OW0	HOH	X	41	20.358	39.276	1.884	1.00	22.25
9364	OW0	HOH	X	42	59.729	80.370	3.839	1.00	25.41
9367	OW0	HOH	X	43	9.394	25.625	7.660	1.00	19.98
9370	OW0	HOH	X	44	19.279	13.591	19.445	1.00	25.74
9373	OW0	HOH	X	45	18.592	28.894	9.372	1.00	21.52
9376	OW0	HOH	X	46	16.733	32.742	-2.993	1.00	17.70
9379	OW0	HOH	X	47	28.337	35.553	9.793	1.00	24.55
9382	OW0	HOH	X	48	71.766	52.024	1.660	1.00	25.10
9385	OW0	HOH	X	49	5.509	18.812	21.857	1.00	25.11
9388	OW0	HOH	X	50	25.249	44.467	-11.635	1.00	22.90
9391	OW0	HOH	X	51	16.089	35.932	-5.867	1.00	20.15
9394	OW0	HOH	X	52	50.870	75.101	10.886	1.00	22.51
9397	OW0	HOH	X	53	58.111	59.051	3.773	1.00	23.52
9400	OW0	HOH	X	54	84.343	49.350	23.069	1.00	19.58
9403	OW0	HOH	X	55	56.087	75.553	13.615	1.00	15.17
9406	OW0	HOH	X	56	19.494	34.654	-1.382	1.00	20.86
9409	OW0	HOH	X	57	8.799	19.400	4.773	1.00	21.44
9412	OW0	HOH	X	58	39.726	12.512	12.694	1.00	37.61
9415	OW0	HOH	X	59	12.786	3.396	7.777	1.00	28.21
9418	OW0	HOH	X	61	33.547	28.085	-16.167	1.00	24.17
9421	OW0	HOH	X	62	60.548	68.421	32.431	1.00	22.66
9424	OW0	HOH	X	63	52.652	63.594	14.580	1.00	21.16

FIGURE 3 (Cont.)DM

A	B	C	D	E	F	G	H	I	J
9427	OW0	HOH	X	64	63.267	78.956	8.228	1.00	23.96
9430	OW0	HOH	X	65	21.674	40.154	-16.591	1.00	19.82
9433	OW0	HOH	X	66	62.524	73.265	19.235	1.00	24.72
9436	OW0	HOH	X	67	50.175	67.476	14.681	1.00	24.07
9439	OW0	HOH	X	68	16.317	24.542	22.592	1.00	24.88
9442	OW0	HOH	X	70	13.596	32.913	1.425	1.00	18.95
9445	OW0	HOH	X	71	33.743	4.683	-9.292	1.00	21.88
9448	OW0	HOH	X	72	84.877	52.105	15.691	1.00	35.89
9451	OW0	HOH	X	73	28.069	7.721	-7.921	1.00	22.28
9454	OW0	HOH	X	74	29.256	1.053	13.166	1.00	28.61
9457	OW0	HOH	X	75	26.790	-1.137	5.597	1.00	33.71
9460	OW0	HOH	X	76	33.840	27.398	-6.991	1.00	26.70
9463	OW0	HOH	X	77	20.039	38.545	-21.843	1.00	59.27
9466	OW0	HOH	X	78	49.910	55.142	25.447	1.00	26.46
9469	OW0	HOH	X	79	9.843	14.477	-1.615	1.00	27.96
9472	OW0	HOH	X	80	36.808	16.350	8.648	1.00	22.19
9475	OW0	HOH	X	81	43.245	14.999	0.753	1.00	22.13
9478	OW0	HOH	X	82	57.361	79.956	11.239	1.00	25.78
9481	OW0	HOH	X	83	9.775	24.342	-1.506	1.00	22.49
9484	OW0	HOH	X	84	68.131	69.501	22.346	1.00	28.17
9487	OW0	HOH	X	85	64.173	83.689	11.530	1.00	19.53
9490	OW0	HOH	X	86	58.920	48.042	6.438	1.00	22.32
9493	OW0	HOH	X	87	57.493	77.168	11.232	1.00	19.16
9496	OW0	HOH	X	88	77.326	71.627	2.643	1.00	27.72
9499	OW0	HOH	X	89	74.547	71.580	7.451	1.00	24.66
9502	OW0	HOH	X	91	48.469	59.380	21.046	1.00	23.24
9505	OW0	HOH	X	92	59.723	83.049	3.647	1.00	26.08
9508	OW0	HOH	X	93	29.853	24.288	-1.800	1.00	33.40
9511	O	HOH	X	94	56.128	56.547	-0.069	1.00	31.76
9514	O	HOH	X	95	60.992	57.155	5.055	1.00	25.17
9517	O	HOH	X	96	57.412	60.876	1.767	1.00	27.49
9520	O	HOH	X	98	10.425	34.341	14.720	1.00	25.28
9523	O	HOH	X	99	58.393	61.924	14.465	1.00	21.57
9526	O	HOH	X	100	15.514	40.203	-8.447	1.00	25.83
9529	O	HOH	X	101	71.395	44.872	6.706	1.00	23.21
9532	O	HOH	X	102	59.088	84.453	1.416	1.00	21.13
9535	O	HOH	X	103	10.805	35.476	2.484	1.00	30.21
9538	O	HOH	X	104	78.675	67.094	-0.168	1.00	30.94
9541	O	HOH	X	105	53.216	69.834	17.573	1.00	21.88
9544	O	HOH	X	106	11.540	21.193	-2.775	1.00	23.63
9547	O	HOH	X	107	56.434	66.036	16.603	1.00	21.18
9550	O	HOH	X	108	53.589	69.002	8.469	1.00	26.03
9553	O	HOH	X	109	22.171	2.588	12.364	1.00	25.07
9556	O	HOH	X	110	77.332	49.094	0.357	1.00	25.35
9559	O	HOH	X	111	33.771	36.319	-2.063	1.00	30.82
9562	O	HOH	X	112	12.214	37.251	-5.519	1.00	20.62
9565	O	HOH	X	113	68.012	47.978	18.112	1.00	22.53
9568	O	HOH	X	114	52.583	66.344	14.741	1.00	24.60
9571	O	HOH	X	115	54.317	78.524	24.510	1.00	28.76
9574	O	HOH	X	116	17.315	3.665	4.180	1.00	31.96
9577	O	HOH	X	117	41.900	14.903	-5.570	1.00	23.73
9580	O	HOH	X	118	25.232	6.606	-7.167	1.00	24.37

FIGURE 3 ~~(Cont.)~~DN

A	B	C	D	E	F	G	H	I	J
9583	O	HOH	X	119	69.198	51.022	2.442	1.00	32.30
9586	O	HOH	X	120	54.454	75.970	7.898	1.00	29.61
9589	O	HOH	X	121	72.835	54.092	-0.028	1.00	28.37
9592	O	HOH	X	122	13.624	16.407	-7.904	1.00	26.27
9595	O	HOH	X	123	52.606	51.548	23.966	1.00	31.75
9598	O	HOH	X	124	64.545	60.261	-5.452	1.00	26.24
9601	O	HOH	X	125	48.485	73.411	29.403	1.00	35.53
9604	O	HOH	X	126	73.394	45.286	22.697	1.00	31.73
9607	O	HOH	X	127	1.619	16.387	23.748	1.00	35.87
9610	O	HOH	X	128	51.331	52.037	31.882	1.00	32.80
9613	O	HOH	X	130	59.702	84.785	5.880	1.00	28.09
9616	O	HOH	X	131	35.875	32.733	-2.230	1.00	41.90
9619	O	HOH	X	132	56.078	68.294	9.410	1.00	23.25
9622	O	HOH	X	133	68.940	88.925	-1.936	1.00	24.65
9625	O	HOH	X	134	66.234	47.041	21.983	1.00	27.75
9628	O	HOH	X	135	61.333	46.476	6.833	1.00	25.98
9631	O	HOH	X	136	67.556	54.792	30.084	1.00	27.45
9634	O	HOH	X	137	40.092	4.846	14.202	1.00	33.56
9637	O	HOH	X	138	6.434	23.324	4.635	1.00	23.23
9640	O	HOH	X	139	53.326	52.199	10.569	1.00	27.46
9643	O	HOH	X	140	16.797	40.699	-15.388	1.00	31.25
9646	O	HOH	X	141	55.505	68.569	5.472	1.00	31.05
9649	O	HOH	X	142	19.829	28.141	-14.550	1.00	32.03
9652	O	HOH	X	143	72.192	80.036	19.386	1.00	26.69
9655	O	HOH	X	144	49.567	62.818	10.675	1.00	36.36
9658	O	HOH	X	145	77.624	80.795	7.572	1.00	30.84
9661	O	HOH	X	146	70.251	84.697	14.333	1.00	29.10
9664	O	HOH	X	147	22.147	28.439	-15.860	1.00	25.06
9667	O	HOH	X	149	13.634	35.572	1.265	1.00	25.62
9670	O	HOH	X	150	82.244	46.629	23.769	1.00	35.68
9673	O	HOH	X	151	63.846	88.990	3.561	1.00	28.36
9676	O	HOH	X	152	64.405	73.293	-9.004	1.00	59.74
9679	O	HOH	X	153	19.585	44.233	-0.968	1.00	31.22
9682	O	HOH	X	154	17.128	12.637	-4.589	1.00	25.38
9685	O	HOH	X	155	5.113	33.908	7.713	1.00	38.08
9688	O	HOH	X	156	30.306	34.937	-7.899	1.00	34.44
9691	O	HOH	X	157	3.129	22.986	-4.541	1.00	39.21
9694	O	HOH	X	158	66.626	69.399	13.372	1.00	23.00
9697	O	HOH	X	159	63.446	57.641	29.205	1.00	27.23
9700	O	HOH	X	160	54.243	50.317	14.175	1.00	34.68
9703	O	HOH	X	161	66.368	78.182	-9.856	1.00	26.10
9706	O	HOH	X	162	53.159	57.048	10.179	1.00	27.95
9709	O	HOH	X	163	44.219	16.007	-6.192	1.00	25.11
9712	O	HOH	X	164	80.589	61.008	18.291	1.00	25.88
9715	O	HOH	X	165	28.989	38.706	2.563	1.00	25.75
9718	O	HOH	X	166	11.238	30.773	0.615	1.00	24.14
9721	O	HOH	X	167	53.608	73.127	12.234	1.00	26.24
9724	O	HOH	X	169	63.586	45.033	14.349	1.00	31.13
9727	O	HOH	X	170	77.596	48.785	23.097	1.00	26.73
9730	O	HOH	X	171	84.848	48.026	14.304	1.00	29.46
9733	O	HOH	X	172	4.265	15.315	11.290	1.00	29.33
9736	O	HOH	X	173	3.381	31.069	16.737	1.00	33.72

FIGURE 3 ~~(Cont.)~~DO

A	B	C	D	E	F	G	H	I	J
9739	O	HOH	X	174	55.238	65.487	7.142	1.00	31.03
9742	O	HOH	X	175	9.341	26.913	-11.288	1.00	29.49
9745	O	HOH	X	176	53.199	53.483	20.584	1.00	32.49
9748	O	HOH	X	177	14.338	14.643	-5.988	1.00	23.99
9751	O	HOH	X	178	38.329	22.112	-11.565	1.00	45.14
9754	O	HOH	X	179	39.337	18.256	2.081	1.00	27.57
9757	O	HOH	X	180	56.191	81.845	4.467	1.00	30.98
9760	O	HOH	X	181	20.859	16.036	-15.248	1.00	24.19
9763	O	HOH	X	182	52.592	52.636	34.412	1.00	33.36
9766	O	HOH	X	183	8.751	22.025	4.991	1.00	21.08
9769	O	HOH	X	184	63.183	88.654	8.668	1.00	32.88
9772	O	HOH	X	185	23.296	39.123	11.088	1.00	28.53
9775	O	HOH	X	186	21.029	42.374	-4.623	1.00	40.24
9778	O	HOH	X	187	61.193	73.706	-5.808	1.00	35.26
9781	O	HOH	X	188	55.468	47.798	19.949	1.00	28.75
9784	O	HOH	X	189	35.734	28.370	-1.891	1.00	42.91
9787	O	HOH	X	190	28.941	9.752	-9.745	1.00	28.83
9790	O	HOH	X	191	60.836	85.243	-5.478	1.00	33.63
9793	O	HOH	X	193	85.606	61.921	11.265	1.00	33.58
9796	O	HOH	X	194	78.387	74.119	-1.722	1.00	50.78
9799	O	HOH	X	195	7.183	30.679	0.916	1.00	33.15
9802	O	HOH	X	196	32.652	28.076	-18.831	1.00	28.06
9805	O	HOH	X	197	53.948	51.530	21.729	1.00	30.16
9808	O	HOH	X	198	3.740	12.442	13.203	1.00	38.10
9811	O	HOH	X	199	81.671	47.299	9.794	1.00	39.29
9814	O	HOH	X	200	76.149	46.441	21.909	1.00	32.74
9817	O	HOH	X	201	61.151	42.663	13.748	1.00	62.81
9820	O	HOH	X	202	54.688	79.719	12.391	1.00	30.29
9823	O	HOH	X	203	51.275	79.190	10.957	1.00	40.83
9826	O	HOH	X	204	14.506	30.823	-3.503	1.00	21.42
9829	O	HOH	X	205	14.195	32.814	-1.332	1.00	19.33
9832	O	HOH	X	206	12.434	31.396	3.683	1.00	16.08
9835	O	HOH	X	207	18.969	32.213	3.765	1.00	20.53
9838	O	HOH	X	208	17.536	34.005	5.600	1.00	16.75
9841	O	HOH	X	209	33.461	39.878	0.879	1.00	48.09
9844	O	HOH	X	210	78.263	66.876	16.527	1.00	37.29
9847	O	HOH	X	211	80.975	67.293	15.894	1.00	39.50
9850	O	HOH	X	212	82.405	67.613	13.856	1.00	46.74
9853	O	HOH	X	213	50.671	57.527	11.069	1.00	40.42
9856	O	HOH	X	214	51.601	55.517	13.513	1.00	33.26
9859	O	HOH	X	215	62.729	54.517	30.771	1.00	40.62
9862	O	HOH	X	216	60.331	52.329	31.300	1.00	52.01
9865	O	HOH	X	217	31.078	32.997	-9.951	1.00	29.54
9868	O	HOH	X	218	33.614	33.829	-1.558	1.00	23.66
9871	O	HOH	X	219	3.882	31.855	12.746	1.00	38.99
9874	O	HOH	X	220	15.840	40.330	-3.855	1.00	26.18
9877	O	HOH	X	221	15.995	38.459	-6.211	1.00	24.53
9880	O	HOH	X	222	63.555	73.039	-4.552	1.00	36.76
9883	O	HOH	X	223	65.686	72.948	-6.046	1.00	30.87
9886	O	HOH	X	224	61.071	89.367	2.768	1.00	33.44
9889	O	HOH	X	225	85.368	50.306	25.290	1.00	39.68
9892	O	HOH	X	226	10.770	31.661	-1.862	1.00	30.59

FIGURE 3 ~~(Cont.)~~DP

A	B	C	D	E	F	G	H	I	J
9895	O	HOH	X	227	67.074	86.090	20.611	1.00	47.90
9898	O	HOH	X	228	72.225	82.393	20.309	1.00	28.15
9901	O	HOH	X	229	23.258	30.948	-19.639	1.00	37.49
9904	O	HOH	X	230	18.514	43.214	-15.138	1.00	25.15
9907	O	HOH	X	231	18.316	39.793	-17.580	1.00	30.27
9910	O	HOH	X	232	18.565	40.376	-20.157	1.00	27.88
9913	O	HOH	X	233	10.124	22.994	6.965	1.00	22.65
9916	O	HOH	X	234	40.682	5.559	16.461	1.00	35.43
9919	O	HOH	X	235	60.087	44.060	7.813	1.00	29.04
9922	O	HOH	X	236	65.753	46.800	19.256	1.00	33.55
9925	O	HOH	X	237	47.350	74.880	26.880	1.00	40.56
9928	O	HOH	X	238	48.590	70.295	28.815	1.00	22.47
9931	O	HOH	X	239	62.111	62.571	-5.691	1.00	41.29
9934	O	HOH	X	240	58.266	75.096	6.385	1.00	20.97
9937	O	HOH	X	241	57.930	77.196	8.555	1.00	21.06
9940	O	HOH	X	242	60.766	78.814	9.905	1.00	24.54
9943	O	HOH	X	243	61.087	78.751	12.516	1.00	17.96
9946	O	HOH	X	244	66.063	45.873	5.892	1.00	30.86
9949	O	HOH	X	245	68.834	44.595	6.140	1.00	27.12
9952	O	HOH	X	246	40.240	21.104	-0.696	1.00	29.77
9955	O	HOH	X	247	54.038	67.321	16.979	1.00	23.18
9958	O	HOH	X	248	6.161	36.828	-2.610	1.00	45.75
9961	O	HOH	X	249	32.414	42.931	-5.770	1.00	26.20
9964	O	HOH	X	250	8.263	18.675	-2.300	1.00	37.46
9967	O	HOH	X	251	57.682	88.576	6.524	1.00	41.67
9970	O	HOH	X	252	9.403	38.851	14.485	1.00	38.72
9973	O	HOH	X	253	7.150	40.262	16.390	1.00	45.72
9976	O	HOH	X	254	53.657	64.735	-1.870	1.00	50.87
9979	O	HOH	X	255	54.909	49.982	11.303	1.00	29.97
9982	O	HOH	X	256	54.469	48.142	15.766	1.00	35.94
9985	O	HOH	X	257	64.819	51.877	25.591	1.00	48.64
9988	O	HOH	X	258	48.466	60.211	34.761	1.00	34.69
9991	O	HOH	X	259	50.594	60.418	33.231	1.00	29.29
9994	O	HOH	X	260	44.303	61.380	23.666	1.00	50.60
9997	O	HOH	X	261	42.915	58.238	26.279	1.00	44.44
10000	O	HOH	X	262	52.554	63.196	6.954	1.00	45.59
10003	O	HOH	X	263	75.789	43.073	11.027	1.00	45.52
10006	O	HOH	X	264	63.099	46.831	5.108	1.00	38.28
10009	O	HOH	X	265	44.196	64.994	15.827	1.00	37.65
10012	O	HOH	X	266	43.951	62.363	16.102	1.00	46.48
10015	O	HOH	X	267	39.222	63.891	21.996	1.00	52.12
10018	O	HOH	X	268	42.850	63.664	23.396	1.00	50.80
10021	O	HOH	X	269	48.526	74.293	31.675	1.00	36.34
10024	O	HOH	X	270	67.670	48.672	31.258	1.00	51.39
10027	O	HOH	X	271	81.199	48.984	16.751	1.00	28.66
10030	O	HOH	X	272	79.911	47.943	14.775	1.00	31.46
10033	O	HOH	X	273	85.017	50.279	19.126	1.00	30.80
10036	O	HOH	X	274	64.657	81.303	10.384	1.00	30.96
10039	O	HOH	X	275	62.329	87.607	6.341	1.00	31.55
10042	O	HOH	X	276	64.640	86.808	5.080	1.00	34.11
10045	O	HOH	X	277	60.179	93.225	8.295	1.00	40.09
10048	O	HOH	X	278	73.593	79.168	1.381	1.00	35.41

FIGURE 3 (Cont.)DQ

A	B	C	D	E	F	G	H	I	J
10051	O	HOH	X	279	74.858	77.325	-0.481	1.00	41.75
10054	O	HOH	X	280	77.068	76.446	0.836	1.00	38.59
10057	O	HOH	X	281	74.159	76.085	-2.785	1.00	31.06
10060	O	HOH	X	282	79.283	78.702	16.390	1.00	38.20
10063	O	HOH	X	283	77.257	76.993	10.420	1.00	32.78
10066	O	HOH	X	284	77.239	78.246	8.067	1.00	37.50
10069	O	HOH	X	285	73.948	68.872	7.682	1.00	33.72
10072	O	HOH	X	286	77.608	62.256	8.543	1.00	45.53
10075	O	HOH	X	287	84.634	47.863	10.649	1.00	33.57
10078	O	HOH	X	288	89.171	59.221	10.145	1.00	51.60
10081	O	HOH	X	289	88.540	58.568	7.606	1.00	57.77
10084	O	HOH	X	290	44.965	73.834	1.582	1.00	48.13
10087	O	HOH	X	291	49.561	81.495	7.222	1.00	45.30
10090	O	HOH	X	292	70.469	68.660	-8.004	1.00	41.08
10093	O	HOH	X	293	81.881	67.174	-2.963	1.00	39.74
10096	O	HOH	X	294	77.288	57.817	-5.855	1.00	32.90
10099	O	HOH	X	295	76.204	60.286	-6.405	1.00	33.62
10102	O	HOH	X	296	72.178	51.978	-1.088	1.00	40.76
10105	O	HOH	X	297	69.367	55.952	-6.441	1.00	41.52
10108	O	HOH	X	298	66.145	60.092	-7.585	1.00	37.64
10111	O	HOH	X	299	58.836	67.727	-7.779	1.00	45.55
10114	O	HOH	X	300	13.363	3.105	-5.157	1.00	38.92
10117	O	HOH	X	301	13.794	2.664	-0.805	1.00	33.87
10120	O	HOH	X	302	15.442	1.396	0.758	1.00	53.73
10123	O	HOH	X	303	17.525	-0.047	0.589	1.00	35.96
10126	O	HOH	X	304	13.277	5.297	-9.056	1.00	41.07
10129	O	HOH	X	305	10.451	8.808	-4.245	1.00	33.55
10132	O	HOH	X	306	11.127	5.641	1.860	1.00	28.72
10135	O	HOH	X	307	17.465	2.139	-2.799	1.00	30.54
10138	O	HOH	X	308	19.535	2.393	-4.513	1.00	33.31
10141	O	HOH	X	309	9.312	12.628	0.396	1.00	37.60
10144	O	HOH	X	310	7.665	11.510	3.549	1.00	34.31
10147	O	HOH	X	311	6.051	11.080	6.071	1.00	39.84
10150	O	HOH	X	312	10.116	7.158	11.883	1.00	33.40
10153	O	HOH	X	313	9.385	9.324	10.796	1.00	36.05
10156	O	HOH	X	314	14.622	2.412	13.739	1.00	31.45
10159	O	HOH	X	315	13.037	2.160	16.038	1.00	41.01
10162	O	HOH	X	316	5.930	10.969	15.786	1.00	34.44
10165	O	HOH	X	317	4.581	9.801	22.907	1.00	46.13
10168	O	HOH	X	318	1.584	18.885	-1.559	1.00	52.72
10171	O	HOH	X	319	37.184	2.115	-2.954	1.00	43.48
10174	O	HOH	X	320	36.733	3.493	-6.561	1.00	45.09
10177	O	HOH	X	321	20.082	0.677	4.712	1.00	26.47
10180	O	HOH	X	322	20.457	8.134	16.042	1.00	46.78
10183	O	HOH	X	323	19.090	10.262	18.888	1.00	37.59
10186	O	HOH	X	324	24.214	25.499	12.581	1.00	29.01
10189	O	HOH	X	325	14.989	39.048	7.973	1.00	31.76
10192	O	HOH	X	326	11.756	39.045	9.415	1.00	50.88
10195	O	HOH	X	327	7.810	36.884	3.543	1.00	43.84
10198	O	HOH	X	328	3.242	25.497	-3.703	1.00	29.56
10201	O	HOH	X	329	1.219	33.875	16.266	1.00	46.56
10204	O	HOH	X	330	1.544	29.687	13.872	1.00	40.23

FIGURE 3 (Cont.)DR

A	B	C	D	E	F	G	H	I	J
10207	O	HOH	X	331	-0.474	27.413	15.144	1.00	54.89
10210	O	HOH	X	332	4.337	28.953	19.199	1.00	36.94
10213	O	HOH	X	333	-1.539	27.356	11.980	1.00	45.30
10216	O	HOH	X	334	-2.107	24.658	12.397	1.00	38.86
10219	O	HOH	X	335	2.398	22.547	20.759	1.00	43.49
10222	O	HOH	X	336	4.084	16.237	25.067	1.00	35.34
10225	O	HOH	X	337	3.978	13.588	25.815	1.00	45.80
10228	O	HOH	X	338	3.094	17.271	27.390	1.00	40.72
10231	O	HOH	X	339	4.241	24.783	21.717	1.00	35.53
10234	O	HOH	X	340	37.329	4.276	7.908	1.00	35.31
10237	O	HOH	X	341	39.684	14.815	17.121	1.00	27.65
10240	O	HOH	X	342	36.317	20.283	10.218	1.00	40.32
10243	O	HOH	X	343	32.070	22.082	3.932	1.00	19.26
10246	O	HOH	X	344	32.703	24.069	5.500	1.00	30.65
10249	O	HOH	X	345	21.195	37.054	0.700	1.00	23.85
10252	O	HOH	X	346	26.360	48.147	-1.801	1.00	37.57
10255	O	HOH	X	347	23.190	43.465	-4.592	1.00	34.90
10258	O	HOH	X	348	18.440	43.181	-3.522	1.00	30.15
10261	O	HOH	X	349	15.607	42.903	-4.850	1.00	31.05
10264	O	HOH	X	350	13.692	44.194	-3.391	1.00	41.66
10267	O	HOH	X	351	31.128	44.045	-7.531	1.00	41.41
10270	O	HOH	X	352	31.689	47.433	-4.627	1.00	30.20
10273	O	HOH	X	353	32.993	49.163	-3.190	1.00	38.18
10276	O	HOH	X	354	27.426	44.095	-10.304	1.00	33.92
10279	O	HOH	X	355	43.796	13.725	3.108	1.00	23.99
10282	O	HOH	X	356	42.070	17.335	1.525	1.00	30.43
10285	O	HOH	X	357	43.287	19.448	0.553	1.00	33.75
10288	O	HOH	X	358	39.828	16.002	5.397	1.00	35.08
10291	O	HOH	X	359	38.165	17.818	4.577	1.00	37.82
10294	O	HOH	X	360	33.950	17.800	-1.148	1.00	45.50
10297	O	HOH	X	361	11.762	24.758	-4.528	1.00	31.90
10300	O	HOH	X	362	3.975	32.061	-8.760	1.00	36.38
10303	O	HOH	X	363	15.528	42.830	-7.772	1.00	35.25
10306	O	HOH	X	364	14.500	29.223	-15.075	1.00	41.38
10309	O	HOH	X	365	32.850	21.982	-18.707	1.00	37.44
10312	O	HOH	X	366	40.592	8.573	-5.209	1.00	37.21
10315	O	HOH	X	367	25.811	11.663	-16.176	1.00	30.06
10318	O	HOH	X	368	26.945	13.028	-17.719	1.00	49.20
10321	O	HOH	X	369	24.479	22.182	-17.748	1.00	49.87
10324	O	HOH	X	370	21.021	17.997	-19.491	1.00	46.80
10327	O	HOH	X	371	23.217	19.367	-20.360	1.00	51.32
10330	O	HOH	X	372	22.674	25.397	-19.288	1.00	43.41
10333	O	HOH	X	373	12.811	20.249	-12.633	1.00	35.30
10336	O	HOH	X	374	55.709	88.998	19.001	1.00	47.10
10339	O	HOH	X	375	54.100	84.683	17.666	1.00	43.29
10342	O	HOH	X	376	48.970	77.908	17.748	1.00	39.82
10345	O	HOH	X	377	41.899	65.707	18.118	1.00	46.67
10348	O	HOH	X	378	48.368	58.949	18.441	1.00	30.58
10351	O	HOH	X	379	48.070	56.991	22.120	1.00	35.54
10354	O	HOH	X	380	47.998	54.800	20.225	1.00	42.38
10357	O	HOH	X	381	50.349	57.710	17.797	1.00	39.16
10360	O	HOH	X	382	32.392	26.723	0.642	1.00	35.35

FIGURE 3 ~~(Cont.)~~DS

A	B	C	D	E	F	G	H	I	J
10363	O	HOH	X	383	30.720	27.097	-2.250	1.00	27.18
10366	O	HOH	X	384	37.015	26.821	2.778	1.00	49.37
10369	O	HOH	X	385	38.443	23.443	3.534	1.00	33.87
10372	O	HOH	X	386	38.669	19.697	6.394	1.00	36.31
10375	O	HOH	X	387	30.186	-3.337	5.179	1.00	43.04
10378	O	HOH	X	388	36.379	2.179	1.556	1.00	42.15
10381	O	HOH	X	389	41.111	3.324	0.448	1.00	36.90
10384	O	HOH	X	390	43.161	2.676	-1.085	1.00	38.66
10387	O	HOH	X	391	62.047	69.399	25.389	1.00	88.66
10390	O	HOH	X	392	64.141	69.344	27.823	1.00	41.19
10393	O	HOH	X	393	58.875	89.405	12.710	1.00	64.96
10396	O	HOH	X	394	52.351	74.162	-4.548	1.00	47.29
10399	O	HOH	X	395	53.730	70.282	-5.715	1.00	55.71
10402	O	HOH	X	396	47.666	76.863	1.325	1.00	34.63
10405	O	HOH	X	397	59.660	75.843	-9.785	1.00	41.09
10408	O	HOH	X	398	62.561	78.886	-9.940	1.00	50.51
10411	O	HOH	X	399	30.260	2.431	-11.763	1.00	34.80
10414	O	HOH	X	400	27.528	3.971	-14.875	1.00	45.91
10417	O	HOH	X	401	33.506	13.418	-15.971	1.00	38.77
10420	O	HOH	X	402	41.028	6.141	-7.128	1.00	49.46
10423	O	HOH	X	403	28.710	29.035	-18.837	1.00	26.44
10426	O	HOH	X	404	29.796	34.872	-15.688	1.00	37.98
10429	O	HOH	X	405	27.243	36.476	-15.645	1.00	37.96
10432	O	HOH	X	406	31.047	35.920	-10.224	1.00	55.58
10435	O	HOH	X	407	33.680	38.851	-7.405	1.00	50.01
10438	O	HOH	X	408	25.402	37.066	-19.531	1.00	37.00
10441	O	HOH	X	409	35.153	33.776	5.764	1.00	48.02
10444	O	HOH	X	410	35.151	34.064	2.494	1.00	34.05
10447	O	HOH	X	411	34.154	30.349	7.013	1.00	44.18
10450	O	HOH	X	412	8.762	37.486	1.397	1.00	38.43
10453	O	HOH	X	413	7.201	35.165	1.535	1.00	41.39
10456	O	HOH	X	414	26.384	40.391	4.437	1.00	36.18
10459	O	HOH	X	415	51.309	51.810	-0.301	1.00	39.62
10462	O	HOH	X	416	29.679	4.776	17.263	1.00	29.29
10465	O	HOH	X	417	28.029	5.806	20.001	1.00	42.73
10468	O	HOH	X	418	20.603	24.902	18.280	1.00	45.48
10471	O	HOH	X	419	56.231	57.185	2.974	1.00	32.25
10474	O	HOH	X	420	53.164	57.686	5.692	1.00	35.05
10477	O	HOH	X	421	65.428	51.862	28.325	1.00	40.33